Profex

Version 3.3
BGMN Backend

September 14, 2014

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1. Introduction

Profex is a graphical user interface for Rietveld refinement of powder X-ray diffraction data. It supports two different Rietveld backends BGMN [1] and FullProf.2k [2]. Profex does not perform any refinement calculations, but it simplifies the use of the Rietveld backends in many ways:

- It displays diffraction patterns.
- It converts pattern files to formats supported by the backends.
- It simplifies setting up control files with databases for crystal structures and instrument configurations.
- It handles file names.
- It summarizes the results and supports export to CSV file format.
- It supports batch processing and parallel processing of several datasets at a time.

Profex runs on Windows, Linux, and Mac OS X operating systems and is available as free software licensed under the GNU General Public License (GPL) version 2 or any later version. The latest version can be downloaded from [3].

2. Installation

2.1. Windows

2.1.1. Profex-BGMN bundle

Since Profex requires a Rietveld refinement backend, a bundle containing both Profex and BGMN is offered for download on the Profex website. Using the bundle is the preferred way of installation if no previous installation is present on the computer. The directory and file structure of the bundle is shown in appendix **??**. The software does not need installation. The downloaded archive can be extracted to any location on the computer. Automatic configuration of Profex will be able to locate the BGMN installation if the relative paths of the BGMNwin and Profex-3.3 folders are maintained. Therefore, it is recommended to copy the entire bundle to the same location on the hard disk, as shown in Fig. 1. Follow these instructions to install BGMN and Profex:

1. Download Profex-BGMN-Bundle-3.3.zip from [3]
2. Extract the bundle to your harddisk (e. g. C:\Program Files)
3. Run Profex by executing the file profex.exe (e. g. C:\Program Files\Profex-3.3\profex.exe)

The file and directory structure of the bundle is explained in appendix A. Profex is also available for download without BGMN. This is the preferred way of installation if BGMN is already installed on the computer, or if previous versions of Profex are to be upgraded. The Profex binary archive does not need installation. Extracting the archive to the local hard drive is sufficient.

If a previous version is installed on the same computer, using a new version will not interfere with the existing installation. Old and new versions can be used at the same time, they will share the configuration options.

2.2. Linux

A binary archive of BGMN for Linux (i686) is available for download on the Profex website [3]. Profex, however, must be compiled from source. It requires a C++ compiler environment and the Qt toolkit version 5 to be installed [4], including header files. Qt version 5.2 or later is recommended. The following Qt 5 modules and header files must be installed:

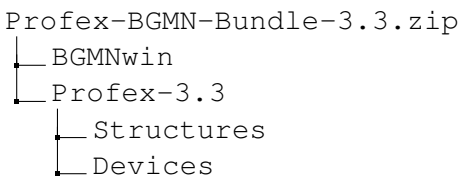
```
widgets, xml, printsupport, script, svg
```

Support for Bruker BRML raw data files requires an additional dependency. The QuaZIP library and header files [5] version 0.4.1 or later must be installed. By default, the Profex source code is configured to include support for BRML files.

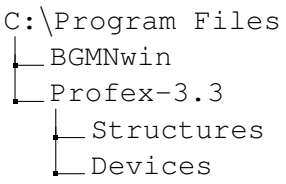
2.2.1. Getting the source

Download the source code archive profex-3.3.tar.gz from the Profex website [3], extract it to your harddisk and navigate into the source code directory:

```
tar xzvf profex-3.3.0.tar.gz
cd profex-3.3.0
```



(a) Structure of the bundle archive.



(b) Structure on the hard disk.

Figure 1: When extracting the Profex-BGMN-Bundle to the hard disk, automatic setup will only be successful if the BGMNwin and Profex-3.3 directories are copied to the same location.

2.2.2. Disabling Bruker BRML support

If BRML support is disabled, Profex only depends on the Qt toolkit. To disable BRML support open the file Profex2.pro in a text editor and change the line

DEFINES += QUAZIP

to

DEFINES −= QUAZIP

Save the file and proceed with the compilation.

2.2.3. Compiling from source code

Run the following commands from the source code directory:

```
qmake Profex2.pro
make -j 4
./profex
```

If error messages occur and the program does not start after typing `./profex`, read the error messages carefully and try to solve all dependency and version problems with your distribution's software repository.

2.3. Mac OS X

A disk image containing Profex and BGMN for Mac OS X 10.6.8 or newer is provided for download on the Profex website [3]. The binary requires a 64bit CPU. Visit [6] to find out whether a specific Apple computer uses a 64bit or a 32bit CPU.

Mount the disk image and drag the folder Profex-BGMN to the Applications folder. The file and directory structure of the bundle is explained in appendix A. Then run the application „Profex-BGMN/profex". The automatic setup routine (section 3) will find the BGMN installation and the structure and device directories.

3. Setup

3.1. Automatic setup

When starting Profex for the first time, the program will try to locate the BGMN installation directory and structure and device database directories automatically. Automatic configuration will also be executed later if the configured paths are invalid. It is therefore possible to force automatic setup later by deleting the paths to BGMN and the database directories in the preferences dialog. Automatic setup is platform specific. The locations scanned automatically are listed below.

3.1.1. Windows

Two directories named „Structures" and „Devices" are expected to be located in the directory of „profex.exe". „BGMN.EXE" is expected to be found in a directory called BGMNwin stored next to the parent directory of „profex.exe", i. e. at:

- `<location of profex.exe>\..\BGMNwin\BGMN.EXE`.

3.1.2. Linux

On Linux, a list of directories is scanned for the executable file „bgmn". Scanning will stop at the first match. The directories are scanned in the following order:

1. `/home/<user>/BGMN/`
2. `/home/<user>/BGMNwin/`
3. `/opt/bgmnwin/`
4. `/opt/bgmn/`
5. `/opt/BGMNwin/`
6. `/usr/bin/`
7. `/usr/local/bin/`

Directories named „Structures" and „Devices" will be searched in the following order at:

1. `/home/<user>/Structures`
   `/home/<user>/Devices`
2. `/home/<user>/BGMN-Templates/Structures`
   `/home/<user>/BGMN-Templates/Devices`
3. `/opt/Structures`
   `/opt/Devices`
4. `/opt/BGMN-Templates/Structures`
   `/opt/BGMN-Templates/Devices`

3.1.3. Mac OS X

On Mac OS X the BGMN installation and Structures and Devices directories will be scanned relative to the path of the Profex application bundle. Profex expects to find the following files, starting at the position of the Profex application bundle:

- `<location of profex.app>/../BGMNwin/bgmn`
- `<location of profex.app>/../BGMN-Templates/Structures`
- `<location of profex.app>/../BGMN-Templates/Devices`

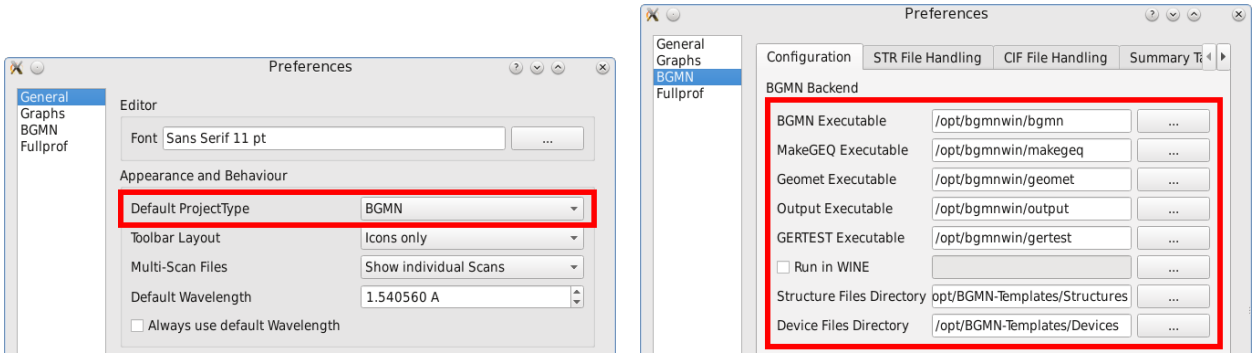
3.2. Manual setup

The following sections describe how to configure Profex to find the BGMN backend, as well as the structure and device database directories manually. There are some scenarios when automatic setup will fail and the backend and database directories are not found, or when the automatic configuration is not desired:

- if only Profex was downloaded instead of a Profex-BGMN bundle
- if the Profex and BGMN folders from the bundle were not copied to the same location on the harddisk
- if Profex is supposed to use existing BGMN and structure/device databases rather than the ones downloaded with the bundle
- on Linux no bundles are available

In these cases, manual configuration is necessary. Follow these instructions to set up Profex manually:

1. Run Profex and go to „Edit → Preferences . . . ".
2. On the page „General" set the „Default Project Type" to „BGMN" (Fig. 2).
3. Go to page „ BGMN". On the tab „Configuration" check the configuration of „BGMN Backend". If auto-detection was successful, the lines for executable files and files directories are not empty (Fig. 2).
4. If the lines are empty, click the button on the right of each line and navigate to the corresponding executable file. The file names depend on the operating system.On Windows, the files are called `BGMN.EXE`, `MAKEGEQ.EXE`, `GEOMET.EXE`, `OUTPUT.EXE` and `GERTEST.EXE`. On Linux and Mac OS X these files are called `bgmn`, `makegeq`, `geomet`, `output`, and `gertest`.



(a) Set the default project type to BGMN.

(b) Select the BGMN executable files, as well as Structure and Device database directories.

Figure 2: Manual configuration of the BGMN backend in Profex.

3.3. Using WINE on Linux

Profex supports running the Windows version of BGMN on Linux using WINE. In that case, a „BGMNwin" directory from a Windows installation can be copied to any location on a Linux system. The executable files of the BGMN backend will then be called `BGMN.EXE`, `MAKEGEQ.EXE`, `GEOMET.EXE`, `OUTPUT.EXE`, and `GERTEST.EXE`. Checking the box „Run in WINE" and entering the WINE executable in the configuration dialog (Fig. 2), which is usually `/usr/bin/wine`, will let Profex call the BGMN backend in WINE. However, for performance reasons it is recommended to use the native Linux version of BGMN if available.

3.4. Structure and Device Database

Profex supports databases for crystal structures and device configurations for the BGMN backend. These databases are directories containing template files. Profex-BGMN bundles are usually shipped with default databases. Profex must be configured to find the database directories. Automatic or manual configuration is explained in section 2.

3.4.1. Structure Template Files

Template files for crystal structures are normal BGMN structure files (*.str) stored at a central place in the „Structures" database directory. The central storage can be placed on a local disk or on a network share, write access is not required for normal use. When appending a structure file from the database to a refinement using Profex's „Add Phase" dialog, the file will be copied to the location of the XRD scan. The original file will never be modified.

The following information is relevant when creating new structure files:

- Use the file extension *.str, other files will be ignored by Profex
- Profex will display the name given after the keyword „PHASE=" in the „Add Phase" dialog.
- It is recommended to add further information, e. g. an original database code (PDF, AMCSD, COD) after a comment sign (`//`) trailing the „PHASE=" keyword (see following example). This text will be shown as a comment in the „Add Phase" dialog.

The following lines show an example of the file „lime.str".

```
PHASE=CaO // 04-007-9734
SpacegroupNo=225 HermannMauguin=F4/m-32/m //
PARAM=A=0.4819_0.4771^0.4867 //
RP=4 k1=0 k2=0 B1=ANISO^0.01 GEWICHT=SPHAR2 //
GOAL=GrainSize(1,1,1) //
GOAL:CaO=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1)
E=CA+2 Wyckoff=a x=0.0000 y=0.0000 z=0.0000 TDS=0.00350000
E=O-2  Wyckoff=b x=0.5000 y=0.5000 z=0.5000 TDS=0.00440000
```

3.4.2. STR File Handling

Depending on where structure files are obtained from (created manually, exported from databases, converted, downloaded, shared with others) they may contain different profile parameters `RP`, `B1`, `k1`, `k2`, `GEWICHT` etc. Altering these files in the structure file database will also affect other users accessing the same database, and may thus not be desired. Profex offers a feature to modify the structure files while copying them from the database to the working directory. Choose „Edit → Preferences → BGMN → STR File Handling" to access the settings (Fig. 3). The individual options on this page are explained in more detail in section 6.3.2.

3.4.3. Device Configuration Files

For each device configuration Profex expects to find four different files in the device database directory. These file names are supposed to have the same file name, but different file extensions (Fig. 4):

***.sav** Containing the description of the device configuration. To be processed with GEOMET.

***.ger** Containing the raytraced profile shape. To be processed with MAKEGEQ.

***.geq** Containing the interpolated profile.

***.tpl** A sample *.sav control file for the refinement, not containing any file names or phases.

The *.tpl file is specific to Profex, all other files will be required by BGMN. The *.tpl file can be any existing refinement control file, but all output file names (`LIST=`, `OUTPUT=`, `DIAGRAMM=`), all scan file names `VAL[n]=`, and all structure file names `STRUC[n]=` should be empty. *.tpl files allow to add goals, calculations, numbers of threads and similar customizations, which will be applied by default when creating a new file set from the database. An example is shown below. All device file names, structure files, scan files, and the various output files will be filled in automatically by Profex. The automatic processes running in the background when using the „Add Phase" dialog are illustrated in Fig. 4. More information on the „Add Phase" dialog can be found in section 7.1.

```
% Theoretical instrumental function
VERZERR=
```

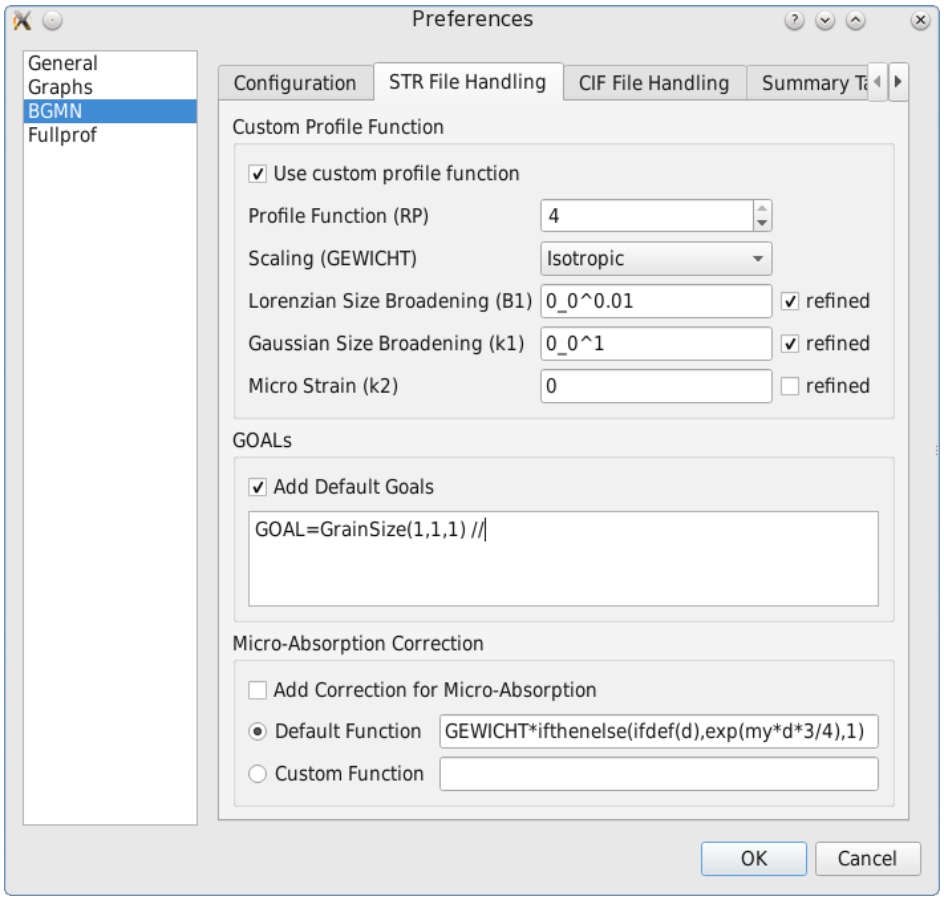


Figure 3: Profex allows to modify structure files automatically to apply custom profile functions and goals.

```
% Wavelength
LAMBDA=CU
% Phases
% Measured data
VAL[1]=
% Minimum Angle (2theta)
% WMIN=10
% Maximum Angle (2theta)
% WMAX=60
% Result list output
LIST=
% Peak list output
OUTPUT=
% Diagram output
DIAGRAMM=
% Global parameters for zero point and sample displacement
EPS1=0
PARAM[1]=EPS2=0_-0.001^0.001
betaratio=0
NTHREADS=2
PROTOKOLL=Y
```

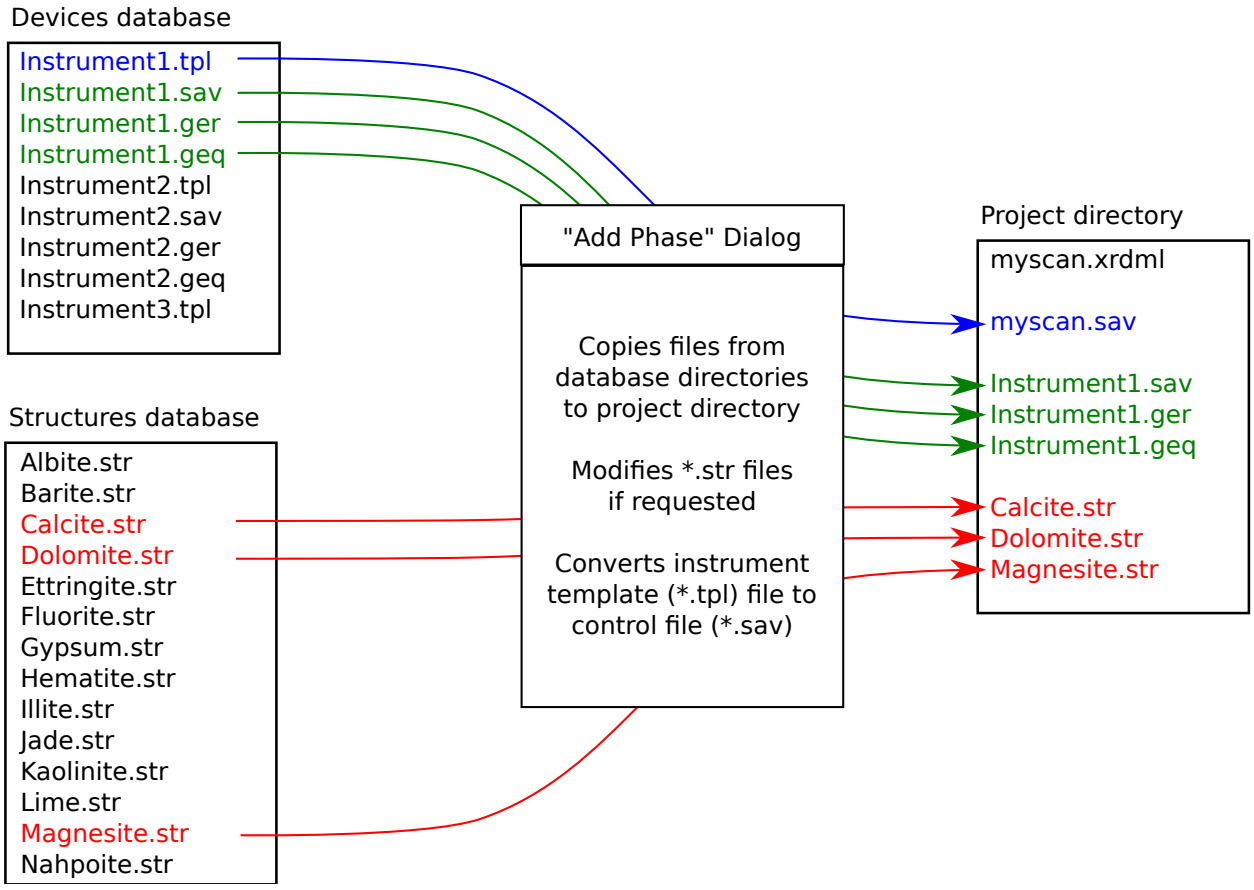


Figure 4: The „Add Phase" dialog will copy structure files and device files from the database directories to the project directory. If selected in the preferences, the structure files will be modified according to the preferences in „STR File Handling". Files already existing in the project directory will not be overwritten, unless the option is checked manually in the „Add Phase" dialog.

4. First steps

When Profex and BGMN have been installed and configured correctly as described in sections 2 and 3, and at least one device configuration and structure file has been stored in the databases (section 3.4), the program is ready for a first refinement:

1. Click „File → Open Graph…", or alternatively press Ctrl+G or the corresponding button in the main tool bar.
2. In the opening file dialog set the file format[1] at the bottom to the format of your raw scan file, and open the file.
3. The scan will be loaded as a new project.
4. Double click on the strongest peak or select a reference structure from the reference structure dropdown menu to identify your main phase.
5. Click „Edit → Add Phase…", or press F8 or the corresponding button in the project tool bar create a control file. The dialog shown in Fig. 9 will be shown.
6. Select your instrument configuration from the dropdown menu, your phase from the structures list (it may be pre-selected), and verify that the option „Generate default control file" is active. Then click „OK".
7. Click „Run → Run Refinement…", F9, or click the corresponding button in the refinement tool bar.
8. Wait for the refinement to complete.
9. If more phases are present, repeat steps 4–7, but make sure the option „Generate default control file" is not active anymore.
10. If the refinement is complete, click „File → Export Global Parameters and GOALs", or press Ctrl+E or the corresponding button in the project tool bar to export the results to a CSV file.
11. Optionally, also click „File → Export Local Parameters and GOALs", or press Shift+Ctrl+E or the corresponding button in the project tool bar to export the local results to a CSV file.

The exported CSV files can be opened in a spreadsheet program such as Microsoft Excel, LibreOffice Calc, or Softmaker PlanMaker. Specify the semicolon „;" as field separator and use the spreadsheet program's sort feature to sort the parameters as needed.

[1] Profex supports a large number of raw data formats. If a format is not supported, or support is broken, other software such as PowDLL [8] is required to convert the scan to a format supported by Profex.

5. Main Window

The program's main window features a menu bar and several tool bars to access all functions and settings (Fig. 5). The central area of the main window is occupied by the plot area, and optionally one or several text editors, which are accessible by tabs at the top of the plot area. The plot area cannot be closed, but text editors can be closed by clicking the close button on their tab.

The central area is surrounded by several dockable windows showing additional information and giving access to more features. These dockable windows can be closed and opened from the „Window" menu. They can also be re-arranged (Fig. 6) by clicking on the title bar showing the window's name, and dragging it to another location. Dockable windows can be stacked on top of each other to hide less frequently used windows, or detached from the main window, e. g. to be placed on another screen, or closed.

5.1. User Interface Elements

The following list explains the elements of the user interface shown in Fig. 5 in more detail.

1 Menu bar gives access to most features, as well as the program's preferences. All menu items are discussed in section 5.6.

2 Main tool bar gives access to file operating features such as opening, saving, etc.

3 Project tool bar gives access to project related functions, such as opening/closing structure files, exporting results, adding/removing phases etc.

4 Refinement tool bar gives access to starting/stopping refinements or batch refinements.

5 Reference structure tool bar allows to select reference structures to display *hkl* indices, as well as to start scanning and indexing new structure files. See section 5.5 for more information.

6 Plot area displays raw or refined scans, and opens text editors for control files, results files, structure files, or generic text files.

7 Projects window lists all open projects and the refinement status. Selecting a project from this list will show it in the central plot area.

8 Plot options lists all scans loaded in the plot area. The „Show" checkbox can be used to show/hide certain scans to customize the appearance of the plot.

9 Refinement protocol shows output generated by the refinement backend.

10 Global Parameters and GOALs shows a summary table of refined global parameters. Listing EPS parameters can be configured in the program's preferences dialog.

11 Local Parameters and GOALs shows a summary table of refined local parameters. The parameters shown here can be customized in the program's preferences dialog.

12 Context help shows the context help text when pressing „F1" on a keyword in a control file.

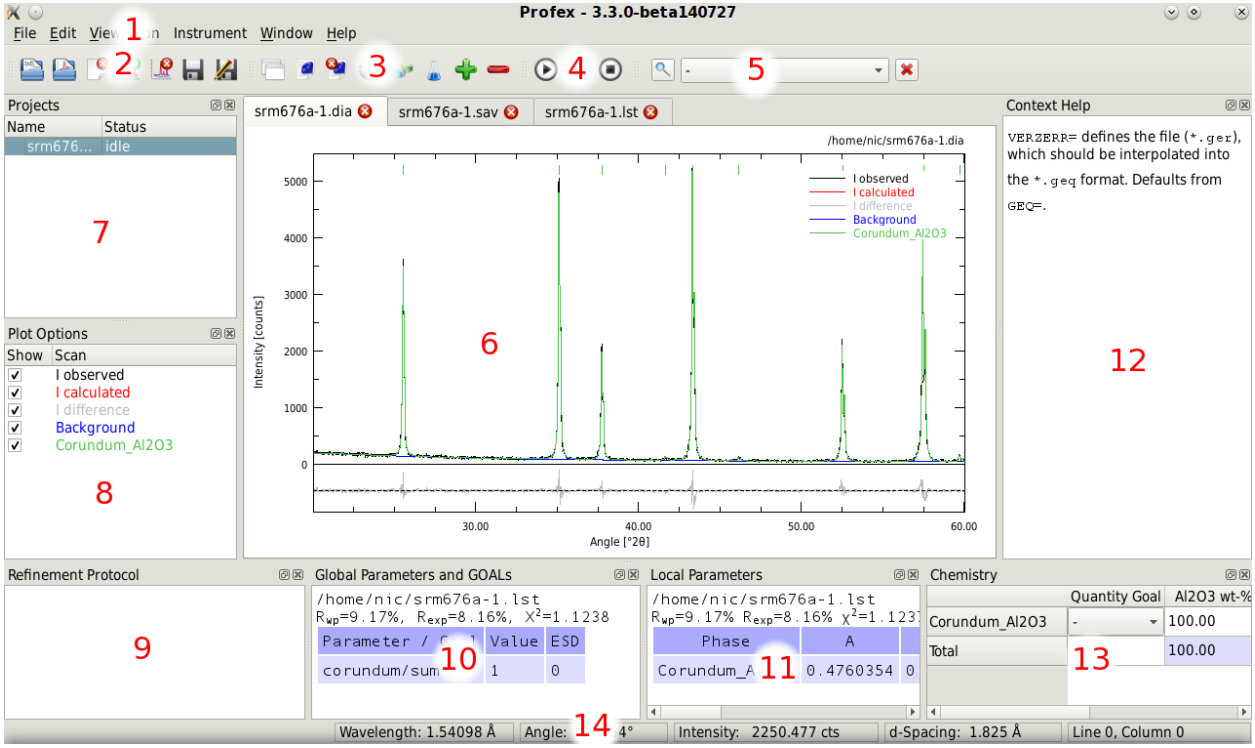


Figure 5: The Profex main window. Elements 1–14 are described in section 5.1.

13 Chemical composition shows the bulk chemical composition of all crystalline phases, calculated from refined crystal structures and phase quantities.

14 Status bar shows various information such as mouse cursor coordinates on the graph, and the wavelength used to transform 2θ angles to d values.

5.2. Dockable windows

All windows arranged around the central plot and editor area (no. 7–13 in Fig. 5) can be rearranged or closed to match the user's preferences. They are called dockable windows, because they can be docked to different areas of the main window. Some examples are shown in Fig. 6 and explained below:

Moving: Grab the dockable window at it's title bar (e. g. the bar (green rectangles on Fig. 6) and drag it to a different location. If the window can be docked, the area will be highlighted.

Stacking: Drag the dockable window onto another dockable window. The dragged window will be stacked on top. Tab buttons will automatically appear to give access to both windows. Unlimited numbers of windows can be stacked.

Detaching: Drag a window outside of the main window and release it when no dockable area is highlighted. The window is now detached from the main window and floating freely on the screen. Use this configuration to place windows on a second screen. Detached windows can also be stacked. Drag the detached window back into the main window to dock it.

Closing / Opening: Dockable windows can be closed by clicking on the close button (x) in the title bar. To open it again, use the menu „Window" in the main window's menu bar.

5.2.1. Projects

This list shows all open projects and their current status. Click on a project to view it in the plot and editor area. Most actions from the menu and toolbar will apply to the currently shown project.

Projects can be edited while another project is refining. Multiple projects can be refined at a time, but refinement may be slow depending on CPU power and number of CPU cores.

Running a batch refinement (see section 5.6.4) will allow to refine all open projects in a sequence, rather than parallel.

5.2.2. Plot options

This list shows all scans loaded in the currently shown project. To change the scans' drawing style (color, line style, line width), refer to the graph preferences discussed in section 6.2. Names of scans cannot be changed, they depend on the names read from the scan files.

Visibility of each scan can be changed by checking or unchecking the box in front of the scan name. For refined scans Profex distinguishes between main scans (usually I_{obs}, I_{calc}, I_{diff}, and the background curve), as well as phase patterns. All phase patterns can be toggled on or off at once by using the function „View → Show/Hide phase patterns". This change is persistent and applies to all open projects. It is a convenience function for easy showing or hiding all phase patterns, but the same result can be obtained by manually checking or unchecking all phase patterns of all open projects.

hkl tick marks are considered as part of phase patterns. Showing/hiding a phase pattern will also show or hide the phase's *hkl* lines. By using the functions in „View → Plot" (see section 5.6.3), drawing of *hkl* lines and phase patterns can be controlled separately. This allows to draw either no phase information, *hkl* lines only, phase patterns only, or both.

Scans can be added or removed to the project by the functions „File → Insert Graph File…" and „File → Remove Scan…". However, as soon as the main graph file is reloaded, for example automatically during a refinement, and added or removed scans will be reset and only the content of the reloaded file will be shown.

5.2.3. Refinement protocol

This windows shows the output of the Rietveld refinement backend.

5.2.4. Global Parameters and GOALs

At the end of the refinement, this window shows a summary of the refinement results. The displayed parameters depend on the Rietveld refinement backend. For BGMN, the table shows all global goals and parameters, including estimated standard deviations (ESD) as calculated by BGMN. Some configuration options are available in the preferences as described in section 6.3.4. Values summarized here can also be exported to a CSV table using the function „File → Export Global Parameters and GOALs (Ctrl+E)" (see section 5.6.1).

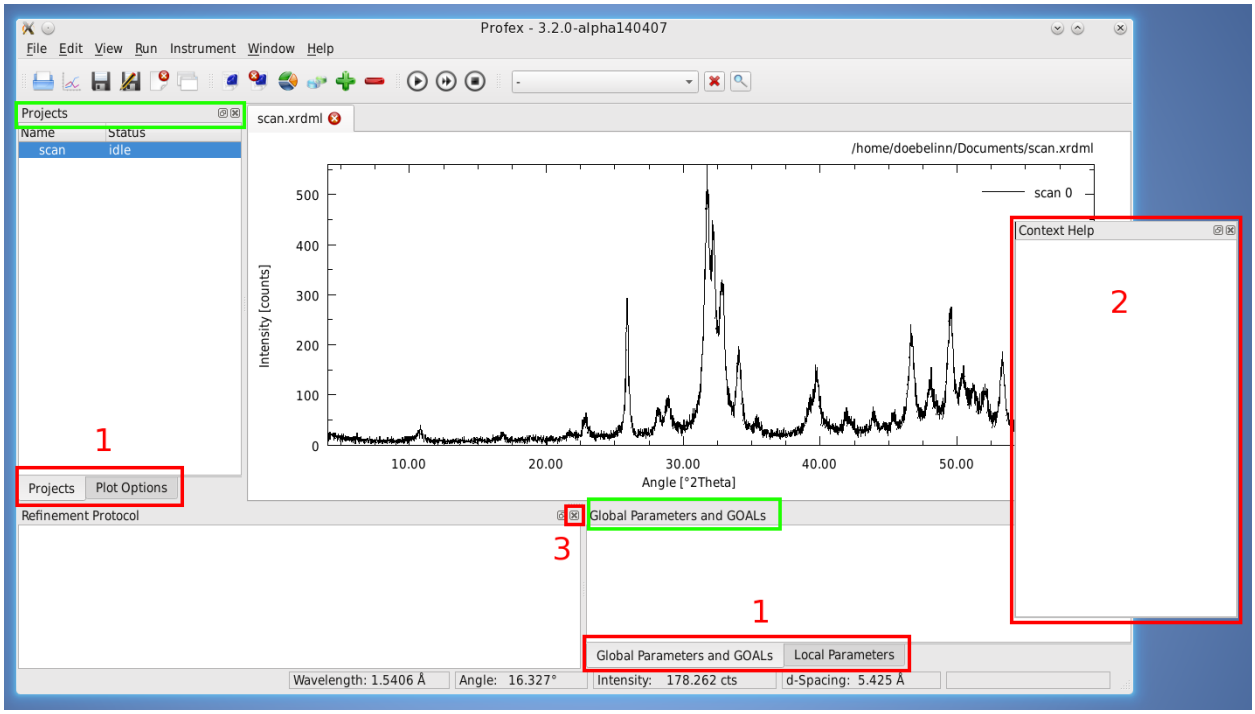


Figure 6: Many elements of the user interface can be re-arranged by grabbing the title bar and dragging the window to a different place (1 stacked; 2 detached from the main window; 3 closed). Green rectangles show the title bars that can be grabbed with the mouse to rearrange the windows.

5.2.5. Local Parameters

At the end of the refinement, this window shows a summary of refined local (phase related) parameters. This function depends on the Rietveld refinement backend and is not available for all backends. In case of BGMN, is is available and can be configured in the preferences as described in section 6.3.4. Values summarized here can also be exported to a CSV table using the function „File → Export Local Parameters" (see section 5.6.1).

5.2.6. Chemistry

The „Chemistry" dock window shows the refined chemical composition of the sample. This information is only available for BGMN, but not for other Rietveld refinement backends. See sections 9 for more information.

5.2.7. Context Help

This window shows the context help, which can be accessed by placing the mouse cursor on a keyword in a control file, and pressing „F1". Context help is available for BGMN, but may not be available for other Rietveld refinement backends (see section 5.6.7).

5.3. The Plot area

The plot area is the central area of the main window. It shows the loaded scans. Some appearance options can be configured in the preferences dialog as described in section 6.2. Visibilities of the legend, *hkl* indices, and phase patterns can globally switched on or off in the menu „View → Plot", as described in section 5.6.

The plot area interacts with the following mouse and key operations:

Moving the mouse cursor: The cursor position will be displayed in the status bar at the bottom of the main window. The horizontal and vertical position will be shown in degrees 2θ and counts or counts per second, depending on the unit of the y-axis (see section 6). Additionally, the horizontal position will also be shown as d value in $\AA$. The wavelength is used to calculate d values. If no wavelength information is found in the scan file, Profex will use the default wavelength specified in the preferences (see section 6).

Hovering the mouse pointer on a *hkl* index line at the top of the plot will show a tool tip displaying the phase name, *hkl* Miller indices, and the texture factor.

Zooming: Use the left mouse button and drag the mouse to zoom the plot. Alternatively, use the mouse scroll wheel to zoom horizontally to the location of the mouse cursor.

Unzooming: Click with the right mouse button to view the entire scan range.

Cross hair cursor: Hold the Ctrl key on the keyboard to show a cross hair cursor.

Counting noise cursor: Hold the Shift key on the keyboard to show a cursor indicating a range of

$$\pm \frac{1}{\sqrt{Intensity[counts]}}$$

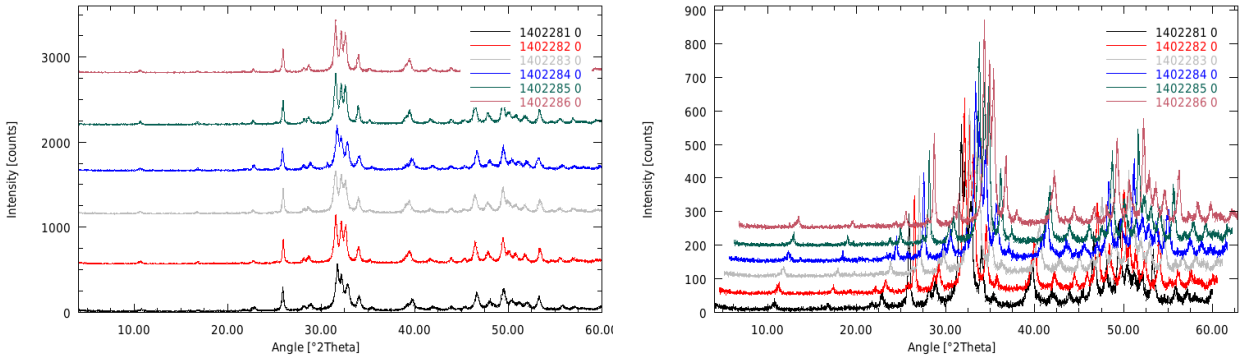
This range represents the statistical counting noise and allows to evaluate mismatches between I_{obs} and I_{calc}, for example at the tips of peaks.

When moving to the difference curve, the noise cursor will show the counting noise at the intensity of the first scan (e. g. I_{obs}) at the same 2θ position.

Load reference structure: Double click with left mouse button will load the reference structure with it's strongest peak closest to the double click position. This is a very primitive way of phase identification, however, it can be very efficient and useful in some situations. Note that only indexed structure files are considered. Refer to section 5.5 for more information on indexing of references structure files. Also note that the strongest peak of the reference structure indices depends on the instrument configuration used for indexing (FDS vs. ADS) and may therefore not be at the location of the currently processed scan.

List of coordinates: Hold the Ctrl key and double click with the left mouse button to copy the coordinates of the mouse cursor to the refinement output console. From there the coordinates can be copied and pasted to another program for further processing.

Scans from different graph files can be added to the plot area by the function „File → Insert Graph File…". Several files can be selected at a time. To remove a specific scan, select it in the



(a) (b)

Figure 7: Vertically (a) and both vertically and horizontally stacked scans (b).

dock window „Plot Options" and click „File → Remove scan…". When starting a refinement, the project's main graph file will automatically be reloaded and all added or removed scans will be reset to the main graph file's content.

5.3.1. Stacking Scans

All scans in the plot area, originating from a single graph file or combined from several graph files using „File → Insert Graph File…", can be stacked vertically and/or horizontally. Offsets can be adjusted by „View → Increase vertical displacement", „View → Decrease vertical displacement", „View → Displace left", and „View → Displace right". All displacements can be reset by „View → Reset Displacement". An initial offset will be applied, which can be reduced incrementally by calling the function moving the scans in the opposite direction. The following commands were used to create the graphs shown in Fig. 7:

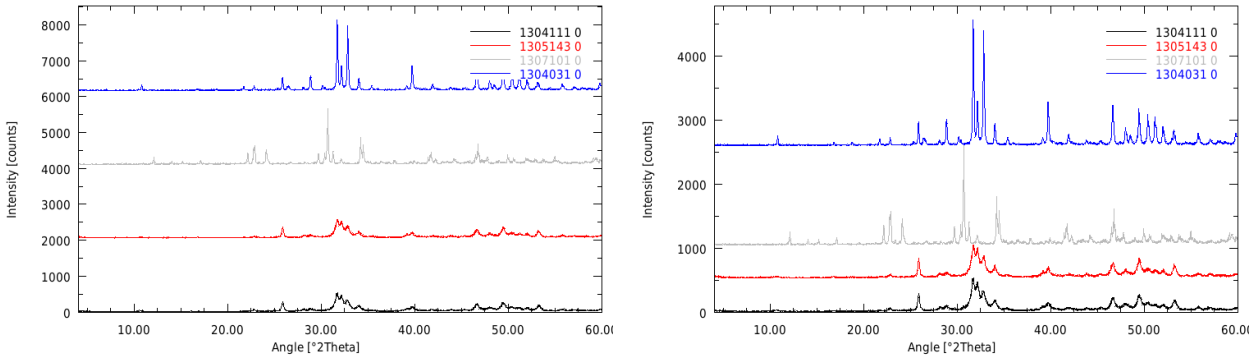
1. „View → Increase vertical displacement" to stack the scans vertically at regular intervals of the maximum intensity of the strongest scan (Fig. 7a).

2. „View → Decrease vertical displacement" was called several times to reduce – not reset – the vertical offset, followed by „View → Displace right" to stack the scans to the right (Fig. 7b).

A special vertical offset will be applied when calling „View → **Decrease** vertical displacement" **first**. In that case, positive vertical stacking will be applied, but instead of regular intervals, each scan will be displaced to the maximum intensity of the previous scan (Fig. 8). This will avoid large gaps above scans with low maximum intensity, however, it can also be confusing with scans of very low intensity (e. g. amorphous samples or the background curve). In the latter case, applying a regular stacking interval by calling „View → **Increase** vertical displacement" may be preferred.

5.4. Text Editors

Text editors can show any kind of text files, including control files, list files, structure files, or any generic text file. For control files and list files they will show syntax highlighting for better visual orientation.



(a) Regular offset

(b) Adaptive offset

Figure 8: When starting with no offset, calling „View → **Increase** vertical displacement" will apply an even offset of the maximum intensity of the strongest scan (a). Calling „View → **Decrease** vertical displacement" will apply an adaptive offset, each scan will be placed at the maximum intensity of the scan below (b).

Besides the standard actions for text editors, such as copy, paste, undo, redo, and selection, the context menu shown by clicking with the right mouse button has some special features for control and structure files.

5.4.1. Control Files

Open File: When placing the cursor on a file name and clicking with the right mouse button, the context menu will show the action „Open File" at the bottom. Depending on the file type, the file will be opened as a scan file (VAL[n], DIAGRAMM), or as a text file (STRUC[n], STRUCOUT[n], SimpleSTRUCOUT[n], RESOUT[n], PDBOUT[n], FCFOUT[n]).

Note that if the file name contains spaces or underscores, the file name must be selected before right-clicking. Else the file name will not be recognized correctly.

5.4.2. Structure Files

When placing the cursor on a parameter and clicking with the right mouse button, the context menu will offer the following actions:

Fix Parameter: This will set the parameter under the mouse cursor to be fixed.

Refine Isotropically: This will release the parameter under the mouse cursor for isotropic refinement. Reasonable lower and upper limits will be applied by default.

Refine Anisotropically: This will release the parameter under the mouse cursor for anisotropic refinement. A reasonable upper limit will be applied by default. Note that if the parameter cannot be refined anisotropically (e. g. unit cell parameters, fractional coordinates, etc.), this option will not be available.

5.5. Tool bars

All functions shown in the main toolbar, project toolbar, and refinement toolbar are also accessible in the menu bar and are described in detail in section 5.6. Toolbars can be re-arranged by dragging the left end to another position, or shown / hiden by right-clicking on a toolbar and checking or unchecking the toolbar in the context menu.

Elements of the reference structure toolbar are only visible if at least one project is loaded. They are not accessible through a menu, only by the toolbar buttons:

Reference structures: A menu allowing to select a reference structure from all STR files found in the structure database directory. If selected, the STR file's *hkl* lines will be shown in the graph. This is a generic way of phase identification. When using the ,,Add Phase" dialog while a reference structure is displayed, this structure file will be pre-selected in the ,,Add Phase" dialog.

If STR files have not been indexed before, *hkl* indices will be calculated on the fly when the structure is selected. On modern computers, this only takes a second or two. Afterwards the *hkl* positions will be buffered and be available instantly. The buffer can be cleared as described in section 6.1.3. Note that the double-click function described in section 5.3 is only available for indexed reference structures.

Reset reference structure: This button will reset the reference structure dropdown menu and hide reference *hkl* lines. After resetting, no structure will be pre-selected in the ,,Add Phase" dialog anymore.

Search and index new reference structures: Pressing this button will scan the structure database directory for new STR files and index all new files. The reference structures become immediately available in all projects.

5.6. Menu Structure

5.6.1. File

Open Text File...(Ctrl+O) Opens a file in a text editor. If a project with the same name as the text file's base name is already open, the file is opened in this project. Else a new project is created.

If the text file is a control or results file, Profex will automatically locate all other control and results files of the same project, as well as the scan file, and open them, too. Non-existing files are ignored.

BGMN structure files (*.str) are always opened in the currently shown project, regardless of the project name.

Open Graph File...(Ctrl+G) Opens a scan file in the graph page. If a control and/or results file with the same base name is found, Profex will open it, too.

Insert Scans...(Ctrl+I) Inserts scans from one or more graph files into an existing project. The additional scans will only be displayed in the project's graph view. Other files, such as the control file, will not be modified. If no project is available, a new one will be created,

based on the name of the first selected graph file. Inserted scans will be discarded when the project's graph file is reloaded, e. g. during a refinement.

Remove Scan... Removes the scan selected in the „Plot Options" window from the graph view. No other files will be modified. Removed scans will be restored when the project's graph file is reloaded, e. g. during a refinement.

Save (Ctrl+S) Saves the current file under the same file name. This function only works for text files.

Save file as... (Shift+Ctrl+S) Saves the current file under a new file name. A file dialog is shown to ask for the file name, location, and file format.

Recent Graph Files Shows a list of recently opened graph files.

Recent Text Files Shows a list of recently opened text files. For scan files, different output formats can be selected. Scans can be saved as raw data for further processing, or images.

Print (Ctrl+P) Prints the currently shown text or graph file. Printing options may differ depending on the platform and device driver.

Close Project (Ctrl+W) Closes the current project.

Open all project STR files Opens all BGMN structure files (*.str) referenced in the current project's control file (*.sav) in new pages.

Close all project STR files Closes all BGMN structure files (*.str) shown in the current project.

Import CIF... Opens a dialog to convert CIF files (*.cif) to BGMN structure files (*.str). See section 11 for more information.

Scan Batch Conversion... Opens a dialog for batch conversion of graph files. All currently opened project scans will be added to the batch list by default. More files can be added or deleted in the dialog. See section 10 for more information.

Export Global Parameters and GOALs (Ctrl+E) Exports the global parameters and goals (e. g. phase quantities) to a semicolon separated spread sheet (*.csv). See section 8.3 for more information.

Export Local Parameters and GOALs (Shift+Ctrl+E) Exports the local parameters and goals (e. g. structural parameters) to a semicolon separated spread sheet (*.csv). See section 8.3 for more information.

Export Chemistry... Writes the calculated chemical composition to a semicolon separated spread sheet (*.csv). See section 8.3 for more information.

Quit (Ctrl+Q) Quits the application.

5.6.2. Edit

Undo Reverts the last change in the currently shown text file.

Redo Restores the last undone change in the currently shown text file.

Copy Control File Copies the current project's control file to other projects and adapts all input and output file names to match the projects' base names. A dialog will allow to select which projects' control file shall be modified. Existing control files will be overwritten.

Note that this function does not check whether referenced structure files are actually present in all project directories. It only manages control files, but not structure files.

Reset File Reverts the current project's control file to the state before the last refinement. This function is only used for the Fullprof.2k backend, but not for BGMN, because BGMN usually does not modify STR and SAV files.

Add Phase... (F8) Opens a dialog to create a control file by selecting an instrument configuration and phases (crystal structure files).

If a phase is activated in the Reference Phase box, it will be preselected in the Add Phase dialog.

The option to create a default control file is automatically activated or deactivated, depending on whether or not a control file already exists.

If a default control file is created despite an existing control file, the existing one will be overwritten, any previously added modifications or phases will be lost.

Selected structure files and instrument configuration files will be copied from the structure and device database directory to the project directory. Files already existing in the destination directory will be skipped. If the option „overwrite existing files" is checked, existing structure files will be overwritten with the file copied from the structure file database. See section 7.1 for more information.

Remove Phase... Removes a phase from the control file. Optionally, the structure file will be deleted. Deleting structure files may cause problems with other projects stored in the same directory and accessing the same structure files.

Preferences... Opens the program's preferences dialog. All preference options are discussed in detail in section 6.

5.6.3. View

Switch to Graphs (Ctrl+1) Raises the Graph page of all projects.

Switch to Control Files (Ctrl+2) Raises page 2 (usually the control file) of all projects.

Switch to Output Files (Ctrl+3) Raises page 3 (usually the results file) of all projects.

Set Zoom Range... Opens a dialog to zoom the graph to precise upper and lower limits for angle and intensity.

Show/Hide Phase Patterns (Ctrl+0) Activates or deactivates visibility of all phases. This option applies to all open projects. It only checks or unchecks the visibility boxes of all phase patterns in the Plot Options list for convenient displaying or hiding of all phases. Individual phases can be shown or hidden by selecting or un-selecting the „show" option in the Plot Options list. More information is given in section 5.2.2.

Plot Configure the visibility of the following elements on the plot:

Phase Patterns Shows or hides patterns of phases.

Legend Shows or hides the plot legend.

hkl Indices Shows or hides the *hkl* index tick marks at the top of the plots.

Increase Vertical Displacement (Ctrl+Up) Applies a regular vertical offset to all scans. The initial offset will correspond to the maximum intensity of the strongest scan. When called again, this function will increase the previous offset by a constant value.

Decrease Vertical Displacement (Ctrl+Down) Reduces the vertical offset of all scans by a constant value. If no vertical offset exists, an initial adaptive offset will be applied, with a vertical displacement of each scan corresponding to the maximum intensity of the scan below.

Displace left (Ctrl+Left) If no horizontal offset exists, it will apply a horizontal offset to the left to all scans. If an offset to the left exists, the offset will be increased by a constant value. If an offset to the right exists, the offset will be reduced by a constant value.

Displace right (Ctrl+Right) If no horizontal offset exists, it will apply a horizontal offset to the right to all scans. If an offset to the right exists, the offset will be increased by a constant value. If an offset to the left exists, the offset will be reduced by a constant value.

Reset Displacement (Ctrl+Space) Resets all horizontal and vertical offsets.

5.6.4. Run

Run Refinement (F9) Starts the refinement of the currently shown project.

Abort (Ctrl+C) Aborts refinement of the currently shown project. In batch refinement mode, all running and scheduled refinements will be aborted.

Run Batch Refinement (F10) Starts a batch refinement of all open projects.

5.6.5. Instrument

Edit Configuration... Opens a dialog to process BGMN instrument configurations. See section 12 for more information.

5.6.6. Window

Projects Shows or hides the Projects list window.

Plot Options Hows or hides the Plot Options window.

Refinement Protocol Shows or hides the Refinement Protocol window.

Global Parameters and GOALs Shows or hides the summary table window for global parameters and goals.

Local Parameters Shows or hides the summary table window for local parameters and goals.

Chemistry Shows or hides the table showing the refined chemical composition in oxide form.

Context Help Shows or hides the context help display.

5.6.7. Help

Context Help...(F1) Shows the context help of the keyword under the text cursor. The ,,Context Help" window (,,View" menu) must be shown to display the context help.

BGMN Variables... Opens a web browser showing the BGMN variables documentation page.

BGMN SPACEGRP.DAT... Opens a dialog to browse spacegroups and atomic positions supported by BGMN.

About Profex... Shows information about Profex.

6. Preferences

6.1. General

6.1.1. Editor

Font Sets the font of the text editor and refinement protocol window.

6.1.2. Appearance and Behaviour

Default Project Type For files not specific for either BGMN or Fullprof.2k, this option determines which type of project will be created when such a file is opened. The file type is identified by the file extension.

File extensions can also be associated with either of the two backends by adding the extension either to the list of „File Extensions associated with BGMN" or „File Extensions associated with Fullprof" on the corresponding backend configuration pages of the preferences dialog.

Toolbar Layout Select how icons and text in Profex' toolbars are shown.

Multi-Scan Files Select whether multi-range files will be shown as individual scans, as the sum of all ranges, or as the average of all ranges.

Default Wavelength This wavelength, given in Å, is used for scan files not containing any information about the wavelength.

Always use default Wavelength If checked, Profex will ignore the wavelength read from the scan file and always use the default wavelength to calculate d values from diffraction angles.

Restore open projects If checked, Profex will load all previously open graph files upon program start.

6.1.3. Reference Structures

Automatically index new structure files If checked, Profex will scan the structure file directory for new structure files each time Profex is started and the first project is loaded.

If not checked, new structures will be indexed the first time they are selected in the Reference Structures box.

Structures will not be available for double-click phase identification as long as they have not been indexed.

Clear Buffer Clears the buffer file with structure file *hkl* indices. Profex must be restarted for this to take effect. All structure files will be re-indexed either automatically, or when selected from the Reference Structures box.

Calculate hkl positions in range Specifies the lower and upper 2θ angle for *hkl* indices to be calculated. Larger ranges will require more time to index. The range may be smaller or larger than scan file ranges.

6.2. Graphs

6.2.1. General Appearance

Use AntiAliasing for Graphs (slow!) Uses anti aliasing to draw the plots. If checked, lines look smoother but also wider. Drawing will be slower if checked.

Update Graph after each Cycle If checked, the plots will be updated continuously during the refinement. If not checked, they will remain static and only be updated at the end of the refinement.

Updating the graph takes some time. For very long refinements or batch refinements deactivating this option may save some time. For normal operation it is recommended to activate this option.

Display Line Width Width in pixels of all lines (plots, axes, tick marks) of the graph on computer screens.

Printing Line Width Width in points of all lines (plots, axes, tick marks) of the graph on printouts. This value should usually be greater than the display line width.

Symbol Size Size of the measured data points when not using solid lines (e. g. dots or crosses) in pixels.

Y-axis Scaling Scaling of the y-axis. Options are linear, logarithmic with a base of 10 (log10), or square root (sqrt).

Color of Reference hkl Lines Color of the *hkl* lines when selecting a reference structure from the Reference Structures box.

Create Thumbnail If checked, a thumbnail picture of the refined plot will be created at the end of the refinement. This file is stored in the project directory with the name `project-basename_tn.png`. It allows easy browsing of refined projects. The width of the picture can be specified in pixels. The height is calculated from the displayed aspect ratio.

Show Texture of hkl Lines (if available) If checked, the box appearing when pointing the mouse cursor on *hkl* index tick marks on the plot also shows the texture factor.

Y-axis unit Shows the y-axis unit either in counts, or in counts per second (cps). Counts per second may not be available, depending on the file format of the loaded scan. If the time per step is not available, Profex will fall back to the unit „Counts" and assume a counting time of 1 second per step.

Only the display of scans will be affected by the choice of the unit. Internally, all calculations and file format conversions will be performed in „Counts". As a consequence, when converting a format supporting „Counts per second" (such as XRDML) to a format not supporting it (such as ASCII XY), the displayed unit may change from [cps] to [counts].

6.2.2. Fonts

Font Title Select the font of the file name at the top-right of the graph.

Font Axis Labels Select the font of the graph axis labels.

Font Tick Marks Select the font of the graph tick marks.

Font Legend Select the font of the graph legend.

6.2.3. Scan Styles

Color Customize the list of colors to be used to draw scans by double-clicking on the color cell. If more scans are loaded than colors are available from the list, a random color will be created and added to the list. It can be changed manually later. Line widths can be changed on the Graph's General Appearance page.

Point Style Select the style to draw scans. „Solid" draws the scan as a solid line. „Points" draws a dot at the measured position, „Cross" draws a cross at the measured position. Symbol sizes of crosses and points can be changed on the Graph's General Appearance page.

+ Add another color to the color list.

− Remove the currently selected color from the list.

6.3. BGMN

6.3.1. Configuration

BGMN Backend

BGMN Executable Select the BGMN executable file. This file is part of the BGMN installation. It is called `BGMN.EXE` on Windows, and `bgmn` on Mac OS X and Linux.

MakeGEQ Executable Select the MakeGEQ executable file. This file is part of the BGMN installation. It is called `MakeGEQ.EXE` on Windows, and `makegeq` on Mac OS X and Linux.

Geomet Executable Select the Geomet executable file. This file is part of the BGMN installation. It is called `GEOMET.EXE` on Windows, and `geomet` on Mac OS X and Linux.

Output Executable Select the Output executable file. This file is part of the BGMN installation. It is called `OUTPUT.EXE` on Windows, and `output` on Mac OS X and Linux.

GERTEST Executable Select the GERTEST executable file. This file is part of the BGMN installation. It is called `GERTEST.EXE` on Windows, and `gertest` on Mac OS X and Linux.

Run in WINE This box is only available on Linux and Mac OS X. It allows to use the Windows version of BGMN to be run in WINE. Check this option if the executable files specified above belong to the Windows version of BGMN.

Structure Files Directory Specify the location where BGMN structure files (*.str) are stored.

Device Files Directory Specify the location where BGMN instrument files (*.sav, *.ger, *.geq, *.tpl) are stored.

File Extensions

File Extensions associated with BGMN These file types will always be opened as BGMN projects, regardless of the default project type.

Convert raw scans to XY format If checked, raw scan files will be converted to ASCII XY free format (*.xy) prior to starting the refinement.

This option must only be disabled if the raw file format is directly supported by the BGMN backend (e. g. *.val, *.rd).

Performance

Number of CPU cores used by BGMN Specifies how many CPU cores will be used by BGMN by adding `NTHREADS=`*n* to the control file. „Automatic" will use all available cores.

6.3.2. STR File Handling

Custom Profile Function

Use custom profile function Check this option if Profex should automatically change the profile parameters of BGMN Structure files (*.str). The files will be modified when they are copied from the structure database to the project directory by calling „Edit → Add Phase…". If this option is disabled, the profile parameters will not be changed.

Profile Function (RP) Specify the `RP=`*n* parameter.

Scaling (GEWICHT) Specify the `GEWICHT` parameter. Choose `SPHAR`*n* for refinement of preferred orientation, or `ISOTROPIC` for untextured samples.

Lorenzian Size Broadening (B1) Specify `B1`, enter `ANISO` for anisotropic crystallite sizes. Check „refine" to refine this parameter.

Gaussian Size Broadening (k1) Specify `k1`. Check „refine" to refine this parameter.

Micro Strain (k2) Specify `k2`, enter `ANISO4` for anisotropic micro-strain. Check „refine" to refine this parameter.

GOALs

Add Default Goals Check this option if a set of default goals is to be added to each copied BGMN Structure file (*.str). Specify the goals in the text field below. Example:
`GrainSize(1,1,1) //`

Micro-Absorption Correction

Add Correction for Micro-Absorption Check this option if a correction for micro-absorption (Brindlay correction) shall be added to each copied structure file.

Default Function If checked, the correction formula is hard coded to a default function.

Custom Function Check this line and enter a custom correction function if a correction formula other than the default one shall be used.

6.3.3. CIF File Handling

CIF to STR Conversion

Upper and Lower Limits for Cell Parameters Specifies the range for upper and lower limits of unit cell parameters to be added automatically to BGMN Structure files (*.str) created from CIF files.

6.3.4. Summary Table

Output Global Parameters and GOALs

List EPS values If checked, refined `EPS`*n* will be shown in the summary table for global parameters and GOALs. Else `EPS`*n* parameters will be skipped.

Output Local Parameters

Text Editor Enter the parameters to be read from the local parameters and goals section in the BGMN List file (*.lst) and shown in the summary table for local parameters and goals. Enter one parameter per line. The parameters must be written exactly as in the list file, including case sensitivity.

Reset Pressing this button erases the text field with parameters and inserts a default set of parameters.

6.4. Fullprof

FullProf.2k options are described in the user manual for Profex using the Fullprof backend.

6.5. Chemistry

The chemistry page allows to edit the oxide forms and their molecular weights used to calculate the elemental composition of the sample. Elements with empty molecular weight, or with molecular weight of 0.0 g/mol, will be ignored. It is recommended to leave the oxide and molecular weight cells of oxygen (element No. 8) empty to suppress display of oxygen as a separate element in the chemistry results table.

A dialog to easily select the oxide form and automatically calculate the corresponding molecular weight can be opened by double-clicking on the element symbol (left column).

Double-clicking an oxide cell (middle column) or molecular weight cell (right column) allows to enter oxide names and molecular weights directly by bypassing the dialog mentioned above.

Element, Oxide, and Molecular Weight table This table holds the oxide formula and oxide molecular weight for each element. Edit the values by double clicking a cell. Double clicking an element cell will open a dialog to determine oxides and their molecular weight. Double clicking any other cell allows direct input of oxide formulas and values.

Reset Resets the table to the internal default values. All customizations will be lost.

7. Adding and Removing Structure Files

7.1. „Add Phase"

One of Profex' central components is the „Add Phase" dialog (Fig. 9). It is accessed by clicking „Edit → Add Phase…", or pressing F8 or the corresponding button on the project tool bar. This dialog is used to easily create or modify the refinement control file. It will automatically add a `STRUC[n]` reference and related GOALs for phase quantification to the control file, and copy the selected STR files from the structure file database to the working directory (Fig. 4). The individual elements of this dialog are described in detail below.

Generate default control file: If this option is checked, Profex will generate a default control file for the selected instrument configuration. If a template file is found (section 3.4), it will be used to create the control file. Else Profex will present a dialog asking for basic information about the instrument configuration. If the option is active, an existing control file will be overwritten. The default state of this option depends on the presence of a previous control file:

- If a control file was found, this function will be unchecked. Manually activating the option will overwrite the existing control file with a newly created default file.
- If no control file was found, this function will be active.

Instrument configurations: This dropdown menu lists all instrument configurations found in the device database directory (section 3.4).

Structures: This list shows all structure files found in the structure file database directory (section 3.4). Clicking on the header of the table („File Name", „Phase", or „Comment") will sort the table in ascending or descending order of the clicked column. Structures which are selected in the first column will be added to the control file. If a reference structure is shown on the main graph, it will be pre-selected in this dialog.

Expand/Collapse: If structure files are organized in sub-directories in the structure database directory, they will be organized in a tree structure in this dialog. Clicking „Expand/Collapse" will expand or collapse all items in the tree structure for easy navigation.

Overwrite existing files: If a selected structure file is already present in the project directory, it will normally not be overwritten. This preserves customized files. Checking this option will force overwriting of existing files. Use this option with care, as other projects accessing the same structure files will be affected, too.

The „Add Phase" dialog will not allow to add the same phase more than once to a control file. If a selected file is already referenced in the control file, it will just be skipped by the dialog. If multiple entries of the same structure file are requested, the control file will have to be modified by hand.

7.2. „Remove Phase" Dialog

The „Remove Phase" dialog, accessed via „Edit → Remove Phase…", is used to remove `STRUC[n]` entries from the control file and update all related GOALs accordingly. If „Delete

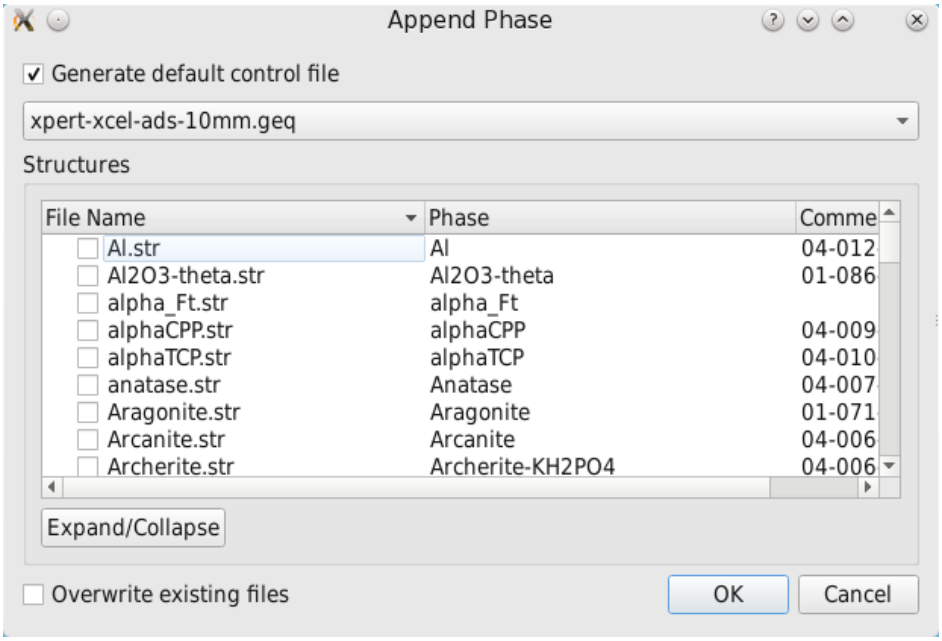


Figure 9: The ,,Add Phase" dialog showing all instrument configuration files and structure files found in the database directories.

STR Files" is selected, the local copies of the selected structure files will be deleted from the hard disk. Note that this can affect other projects accessing the same copies of the structure files. If the control file contains multiple references to the same structure file, only the first occurrence will be removed. In that case, the option ,,Delete STR Files" will be ignored until the last reference to this file was removed from the control file.

7.3. Project organization

When working with several datasets (= projects) at a time, it is important to understand how Profex' ,,Add Phase" function handles structure and instrument files in the background.

By default the ,,Add Phase" dialog will copy selected structure and instrument files to the location of the currently loaded scan file as shown in Fig. 9. It will check whether a file with the same name is already present. If yes, the present file will not be overwritten, unless the option ,,overwrite existing files" was activated for structure files, and ,,generate default control file" was activated manually for instrument files.

Since several raw scan files can be located in the same directory, a structure file will only be present once, even if it was added multiple times for each project. Modifying, removing, or overwriting this structure file will affect all projects within this directory (Fig. 10).

If common structure files are not desired, there are several options to avoid shared access by multiple projects:

- Distribute the raw scans on several sub-directories, as shown in Fig. 10. The ,,Add Phase" dialog will have to be called for each project separately, but each project will receive it's own copy of the instrument and structure files.

- Manually manage the structure files. E. g. create a copy of `structure_1.str` and name it `structure_1a.str`. Then change the `STRUC[1]=structure_1.str` line in the corresponding control file to `STRUC[1]=structure_1a.str`.
- Manually manage structure files by creating sub-directories for structure files only. E. g. create a copy of `structure_1.str` in `strFiles_1/structure_1.str`. Then change the `STRUC[1]=structure_1.str` line in the corresponding control file to `STRUC[1]=strFiles_1/structure_1.str`. The project directory remains unchanged, but it will access the structure files in a specific sub-directory, which can be managed manually for each project.

Projects sharing structure files

```
working directory
├── scan_1.sav
├── scan_2.sav
├── structure_1.str
└── structure_2.str
```

scan_1.sav:
```
STRUC[1]=structure_1.str
STRUC[2]=structure_2.str
```

scan_2.sav:
```
STRUC[1]=structure_1.str
STRUC[2]=structure_2.str
```

Projects in sub-directories

```
working directory
├── dataset_1
│   ├── scan_1.sav
│   ├── structure_1.str
│   └── structure_2.str
└── dataset_2
    ├── scan_2.sav
    ├── structure_1.str
    └── structure_2.str
```

scan_1.sav:
```
STRUC[1]=structure_1.str
STRUC[2]=structure_2.str
```

scan_2.sav:
```
STRUC[1]=structure_1.str
STRUC[2]=structure_2.str
```

Manually renamed structure files

```
working directory
├── scan_1.sav
├── scan_2.sav
├── structure_1a.str
├── structure_2a.str
├── structure_1b.str
└── structure_2b.str
```

scan_1.sav:
```
STRUC[1]=structure_1a.str
STRUC[2]=structure_2a.str
```

scan_2.sav:
```
STRUC[1]=structure_1b.str
STRUC[2]=structure_2b.str
```

Structure files in sub-directories

```
working directory
├── scan_1.sav
├── scan_2.sav
├── strFiles_1
│   ├── structure_1.str
│   └── structure_2.str
└── strFiles_2
    ├── structure_1.str
    └── structure_2.str
```

scan_1.sav:
```
STRUC[1]=strFiles_1/structure_1.str
STRUC[2]=strFiles_1/structure_2.str
```

scan_2.sav:
```
STRUC[1]=strFiles_2/structure_1.str
STRUC[2]=strFiles_2/structure_2.str
```

(a) File structure

(b) Control file content

Figure 10: Projects and structure files can be organized in different ways, depending on whether structure and instrument files shall be shared or not.

8. Exporting data

8.1. Graphs

Scans shown in the plot area can be exported to various formats. Depending on the export format, some information may get lost if it is not supported by the output format. Scans can be exported as follows:

1. Make sure the graph to be exported is shown by selecting the project and showing the „Graph" tab.
2. Select „File → Save File As…".
3. Select the format for the export in the file format dropdown menu.
4. Specify the file name and save the file.

Profex exports some generic file formats, and some formats specific for other applications. The generic formats are useful for most users interested in further data processing or creation of figures. They will be discussed in further detail in the following paragraphs.

8.1.1. ASCII free format (XY)

A generic text format writing the data in columns, starting with the angle, followed by columns with intensities for each scan. These files can be imported in spreadsheet or plotting software for further processing. Spreadsheet software includes Microsoft Excel, LibreOffice Calc, SoftMaker PlanMaker, and others. Plotting software includes OriginLab Origin, GNUplot, and others.

hkl lines will not be exported. Scan colors, line styles, and the legend will also get lost during the export. Visibilities of scans will be ignored, all scans will be exported. A white space character is used for field separation.

The following example shows an exported ASCII free format file with all scans written into one file. The first column contains the x-values (2θ angle), the following columns contain y-values I_{obs}, I_{calc}, I_{diff}, $I_{background}$, and two phase patterns. Note that the phase patterns include the background intensity:

```
4.007500 22.000000 21.070000 0.930000 21.050000 21.050000 21.070000
4.022500 19.000000 20.910000 -1.910000 20.890000 20.890000 20.910000
4.037500 20.000000 20.760000 -0.760000 20.740000 20.740000 20.760000
4.052500 22.000000 20.610000 1.390000 20.590000 20.590000 20.610000
4.067500 24.000000 20.470000 3.530000 20.450000 20.450000 20.470000
4.082500 13.000000 20.330000 -7.330000 20.310000 20.310000 20.330000
...
```

8.1.2. Pixel image (PNG)

Pixel image export will write the file to a Portable Network Graphics (PNG) image. A dialog will open to ask for the output size in pixels. PNG uses lossless compression, therefore relatively small files free of compression artifacts will be created.

If the line width or font size is too small, it will have to be changed prior to the export in the graph preferences (see section 6.2). Use „display line width" to change the export line width.

All elements visible on screen will be exported, including *hkl* lines and the legend. Visibility of the scans will be considered, invisible scans will also be invisible on the exported file. The export will create a high-resolution image of the on-screen graph.

Pixel images can be edited in any photo editing software, such as Adobe Photoshop, GIMP, Paintshop Pro, Corel PhotoPaint, and others.

8.1.3. Gnuplot (GPL)

Gnuplot is a powerful cross-platform graphing utility able to create quality graphs in various formats. Scans exported as Gnuplot files are saved as Gnuplot scripts with inline data. The graphs are a fairly accurate but not perfectly identical representation of the plot as displayed in Profex. It includes *hkl* indices, a legend, all selected scans, and it preserves scan colors and symbol styles. The output file may be edited to optimize the appearance of the Gnuplot graph or to change the output terminal. Gnuplot code created by Profex version 3.3 was optimized for Gnuplot version 4.6.

On a system with a working Gnuplot installation, the following command entered in a terminal emulator will output the graph „scan.gpl" to the default terminal:

```
gnuplot -p scan.gpl
```

8.1.4. Scalable vector graphics (SVG)

Scalable vector graphics (SVG) is a resolution-independent vector graphics format ideal for post-processing of graphs. All elements (scans, axes, *hkl* lines, text) are exported as editable paths or text elements, allowing to change fonts, sizes, places, colors, line widths, or add annotations easily in the exported file. It is the most powerful and flexible of all export formats to create high-quality figures. However, it is necessary to use vector drawing software and convert the format before importing into a word processor, as most programs, including Microsoft Word, LibreOffice Writer, SoftMaker TextMaker, and LaTeX, do not import SVG files directly.

All modern webbrowsers are capable of viewing SVG files natively. SVG files can therefore be viewed and printed easily on all operating systems without requiring any additional software. In order to edit the files, a vector drawing program such as Adobe Illustrator, Inkscape, Corel DRAW, or others is necessary. Note that not all vector drawing programs interpret SVG files correctly. Wrong SVG drawing may need manual optimization.

The recommended workflow to add a scan to a manuscript in high quality is the following:

1. Exort the scan to SVG as described above.
2. Open or import the SVG file in a vector drawing program of your choice.
3. Make sure the SVG file looks as expected. Modify if necessary.
4. Select the entire plot and copy to the clipboard.
5. Special-paste it into the word processor or presentation program, for example as an extended metafile.

8.1.5. Fityk Session (FIT)

Fityk scripts can be opened directly with the program Fityk [9], version 0.9.8 or later. This export filter was specifically designed for phase quantification of calcium phosphate phases for medical devices according to the standard procedure described in ASTM F2024-10. It may not be of much use for anyone not performing this specific analysis.

The Fityk Session export offers several different export modes. „Entire File" will write the entire measured range to a script. All other modes are described in more detail:

Corundum (104) peak: This export mode is to be used with the corundum reference data set. It will export the range from 34.0 to 36.2° 2θ around the corundum (1 0 4) peak. Running the script in Fityk will fit a linear function to the background signal. Afterwards, it will integrate the intensities $I_{obs} - I_{background}$ from 34.4 to 35.9° and print the result. This is the corundum reference intensity to be used for ASTM F2024-10.

b-TCP range: This mode, which is to be used with the CaP data set, will export the range from 27.0 to 35.0° 2θ. Running the script in Fityk will fit a linear function to the background and PearsonVII functions to all peaks except β-TCP (0 2 10), and then integrate the difference between all fitted curves and the observed curve from 30.5 to 31.5° 2θ. This integrated intensity will be used to quantify β-TCP in the sample.

CaO range: This mode will export the range from 36.0 to 38.8° 2θ. Running the script in Fityk will fit a linear function to the background, and integrate the difference $I_{obs} - I_{background}$ from 37.0 to 38.5° 2θ. This integrated intensity will be used to quantify CaO.

HA range: This mode will export the range from 37.5 to 59.5° 2θ. Running the script in Fityk will fit a linear function to the background and integrate the intensities $I_{obs} - I_{background}$ in the range from 38.5 to 59.0° 2θ to quantify hydroxyapatite.

All CaP ranges to separate files: This mode will export all three ranges (β-TCP, CaO, HA) analyzed with the CaP sample to separate files.

8.2. Printing to PDF

On most operating systems a PDF printer is available. It allows direct export of the graph to a PDF file. Prepare the graph as described at the beginning of this section, but use „File → Print…" instead of the save as function. Use the printer dialog to write the output to a PDF file. The layout and functions are platform specific.

If line widths are too fine or too wide, change the printing line width in the preferences, as described in section 6.2. PDF files can be used directly in LaTeX. Other word processors may need the same conversion as described for SVG files.

8.3. Refinement results

At the end of a refinement, Profex shows a summary of global parameters and GOALs, as well as refined local parameters, in the summary dockable windows. These values are read from the LST output file. Local parameters can be customized in the preferences as described in section

File	Sample	Parameter / Goal	Value	ESD
<path>/scan1.lst	scan1	alphaTCP/sum	0.0311	0.0023
<path>/scan2.lst	scan2	alphaTCP/sum	0.0161	0.0022
<path>/scan3.lst	scan3	alphaTCP/sum	0.0147	0.0024
<path>/scan1.lst	scan1	hap/sum	0.9689	0.0023
<path>/scan2.lst	scan2	hap/sum	0.9839	0.0022
<path>/scan3.lst	scan3	hap/sum	0.9853	0.0024

Table 1: Global parameters and GOALS exported from Profex and sorted by the „Paramter / Goal" column. Sorted like this, mean values and standard deviations can easily be calculated.

6.3.4. Profex allows to easily export the global and local refined parameters of all open projects into spreadsheet files:

„File → Export Global Paramters and GOALs" will write the global parameters and goals of all open projects to a CSV file.

„File → Export Local Paramters" will write the local parameters of all open projects to a CSV file.

„File → Export Chemistry" will export the chemical composition (see section 9) to a CSV file.

The exported files are text files containing semicolon-separated fields. Open the file in a spreadsheet program and specify the semicolon character as a field separator. Since the exported files also contain the source file name, using the spreadsheet program's sorting function allows easy sorting and statistical evaluation of the results. The following example shows how the exported CSV file with global parameters and goals looks like if opened in a text editor. Table 1 shows how the same data looks after importing and sorting in a spreadsheet program.

```
File;Sample;Parameter / Goal;Value;ESD
<path>/scan1.lst;scan1;alphaTCP/sum;0.0311;0.0023
<path>/scan1.lst;scan1;hap/sum;0.9689;0.0023
<path>/scan2.lst;scan2;alphaTCP/sum;0.0161;0.0022
<path>/scan2.lst;scan2;hap/sum;0.9839;0.0022
<path>/scan3.lst;scan3;alphaTCP/sum;0.0147;0.0024
<path>/scan3.lst;scan3;hap/sum;0.9853;0.0024
```

9. Chemical composition

After the refinement, Profex will calculate the bulk chemical composition of the sample from the structural information and refined site occupancies reported in the list file (*.lst). The elemental composition, expressed in wt-% of the oxide, is shown in the „Chemistry" dockable widget (Fig. 11). In a first step, Profex will calculate the chemical composition of each phase, and normalize it to 100 % (Fig. 11a). In order to calculate the bulk composition of the entire sample, Profex needs to know the relative quantity of each phase, which is normally calculated as a global goal.

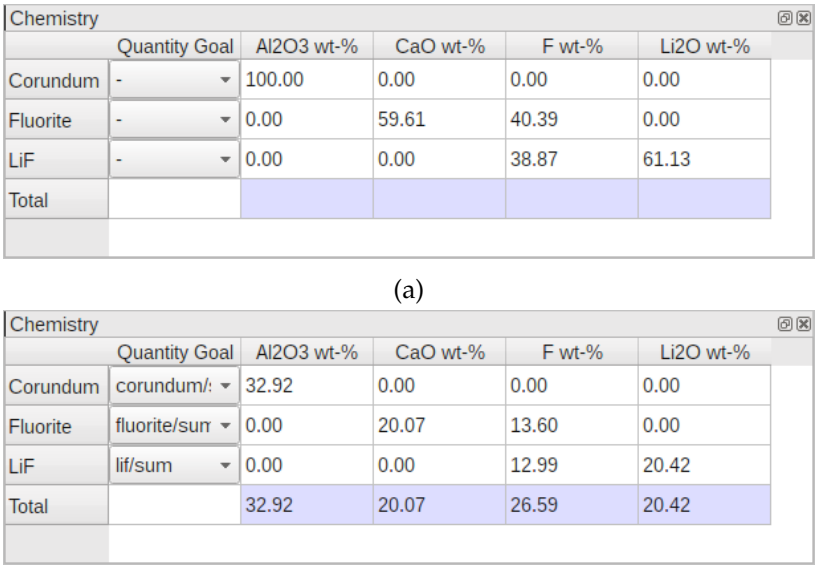


Figure 11: Chemical composition of the sample. Quantity goals must be selected by the user. If no quantity goals were selected (a), each phase will be normalized to 100 %. If the goals describing the phases' quantities were assigned (b), the total bulk composition of the sample will be calculated, too.

Profex will attempt to identify the correct „Quantity Goal" by comparing global goal names with the phase name. If a goal name of format `phase_name/some_string` is found, with `phase_name` matching the phases `PHASE` variable (case insensitive), the goal will be automatically selected. Else no „Quantity Goal" will be selected and the user will have to select it manually.

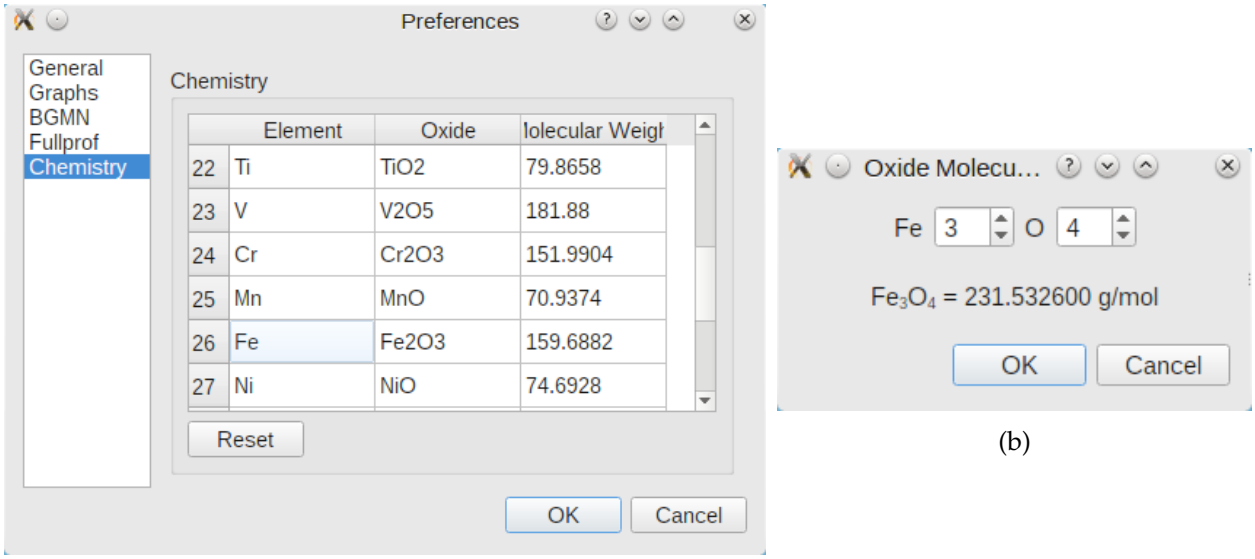
As an example, the following „Quantity Goal" will be recognized and assigned automatically, because the phase name and goal name match (matching is case insensitive):

```
STR file:  PHASE=Corundum
           GOAL:corundum=GEWICHT
SAV file:  GOAL[1]=corundum/sum
```

But the following „Quantity Goal" will not be recognized automatically, because the phase name and goal name do not match. The user will have to select it manually:

```
STR file:  PHASE=Corundum
           GOAL:Al2O3=GEWICHT
SAV file:  GOAL[1]=Al2O3/sum
```

Once a valid „Quantity Goal" has been selected for a phase, the element composition will be normalized to the phase's quantity. The total chemical composition will be calculated only when all phases were assigned a valid „Quantity Goal" (Fig. 11b).



(a) (b)

Figure 12: Oxides and molecular weights can be customized in the preferences dialog (a). Double click on a „Element" cell in the oxide table to open a dialog for calculation of oxide molecular weights (b).

The oxides and their molecular weights used to calculate the composition can be accessed and customized in the preferences by calling „Edit → Preferences… → Chemistry" (Fig. 12a). Elements without molecular weight value, or with a value of 0.0, will be ignored for the calculation. It is recommended to leave the molecular weight of oxygen (element No. 8) empty or at 0.0 to avoid listing oxygen as a separate element in the chemistry output table. See section 6.5 for more information on customizing the oxide parameters.

Select „File → Export Chemistry…" to export the data to a csv file.

10. Scan batch conversion

Several scan files can be converted to other data formats at a time using the „File → Scan batch conversion…" feature. However, due to limitations given by the formats, SVG and pixel images (PNG) are not available for batch conversion.

When opening the batch conversion dialog by clicking „File → Scan batch conversion…", the file queue will contain all currently opened scan files by default. More files can be added by clicking the „Add File" button and selecting one or more files, and selected files can be removed from the queue by clicking the „Remove File" button.

Some output format support multiple scans stored in a single file. The option „Write scans to one file" will instruct Profex to store all scans found in a source file into one single file. In that case, all scans I_{obs}, I_{calc}, I_{diff}, $I_{background}$, and all sub phase patterns found in a DIA file will be stored in a single output file. Use „Write scans to individual files" to write these patterns into single output files instead. Note that storing multiple scans in one file must be supported by the output format as well as by Profex' output filter, which is currently only the case for ASCII and Gnuplot files.

Click „Convert" to start the conversion process, or „Close" to close the dialog without conversion. Output files will be stored at the location of their source files using the same base file name. Existing output files will be overwritten without warning.

11. CIF import

Crystal structure files retrieved from online or commercial databases are usually supplied in the CIF format [7]. Before they can be used with BGMN, the structure information needs to be converted the the BGMN STR file format. Profex provides support to facilitate the conversion process. However, due to incomplete CIF information, many STR files converted from CIF need manual revision.

The following instructions show how to convert a CIF file to a BGMN STR file using Profex' CIF import feature.

1. Retrieve a CIF file from an external resource (online or local database).
2. Start Profex and choose „File → Import CIF…" to open the CIF file.
3. If no space group number was found in the CIF file, Profex will display a dialog to select the number (Fig. 13a). Select the space group number of your structure. It has to be known or determined from an external source. The field „Supported Settings" shows all Hermann Mauguin symbols of the selected space group number. The correct number must contain a symbol remotely similar to the symbol read from the CIF file. Due to the lack of standardization, CIF and BGMN Hermann Mauguin symbols often look similar, but not identical.
4. If more than one space group setting is available, select the correct one from the dialog shown in Fig. 13b. Again, the available Hermann Mauguin symbol often looks similar but not identical to the one read from the CIF file.
5. The STR file will be created and shown in an editor (Fig. 14). Most likely the STR file is incomplete due to information missing in the CIF file. Some warnings are issued in the dialog. Check manually for complete information. Typically Wyckoff sequences and element types are often missing.

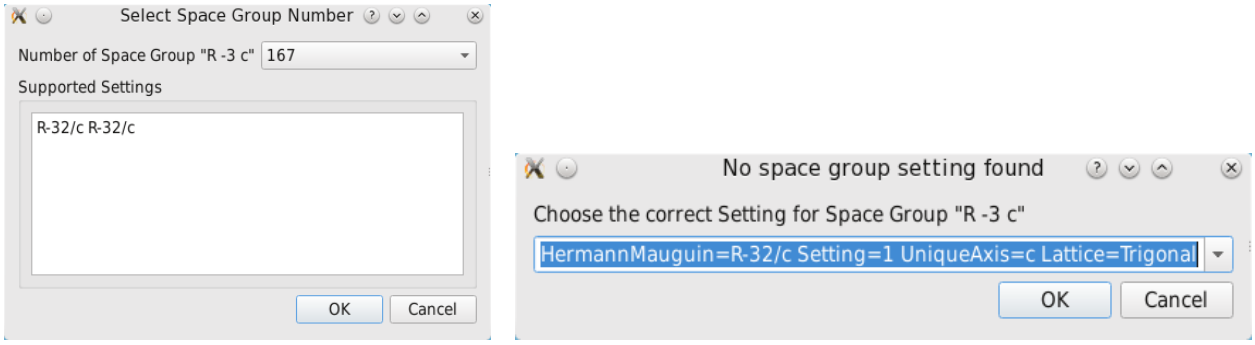
   The dialog also shows the original CIF file on a second tab. It may be useful to verify the STR file or to retrieve more information if it was not extracted automatically. The XML file shown on the third tab is the intermediate format used by Profex. It is only shown for debugging purposes.
6. Once the STR file is complete, choose „Save STR" to save the file in the structure file database directory.

Sometimes it is helpful to browse the space group numbers and symbols in the form supported by BGMN. Open „Help → BGMN SPACEGRP.DAT" to open a dialog which shows all space group numbers, settings, and Wyckoff sequences in the nomenclature used by BGMN (Fig. 15).

The assignment CIF file tags to STR parameters is described in Table 2.

11.1. Automatic conversion of thermal displacement parameters

During the conversion from CIF to STR format Profex automatically transforms the thermal displacement parameters to the format supported by BGMN. Depending on the source format, the following conversions are calculated (anisotropic β_{ij} values are not supported by the CIF format.):



(a) Space group number (b) Space group setting

Figure 13: Importing a CIF file: If no space group number is found in the CIF file, it has to be entered manually in dialog (a). If more than one setting for the space group is available, it has to be choosen manually from dialog (b).

Isotropic B: Isotropic B is the format supported by BGMN. However, BGMN uses a different unit than normally provided in the CIF file. Automatic conversion therefore performs the following conversion:

$$B_{iso}[nm^2] = 0.01 \cdot B_{iso}[\mathring{A}^2]$$

Anisotropic B_{ij}: Anisotropic B_{ij} are converted to isotropic B values in the expected unit [10]:

$$B_{iso}[nm^2] = 0.01 \cdot \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* A_i A_j$$

with reciprocal lattice parameters $a^*[\mathring{A}^{-1}]$ and real lattice parameters $A[\mathring{A}]$.

Anisotropic U_{ij}: Anisotropic U_{ij} are converted to U_{equiv} using the expression [10]:

$$U_{equiv} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* A_i A_j$$

with reciprocal lattice parameters $a^*[\mathring{A}^{-1}]$ and real lattice parameters $A[\mathring{A}]$. U_{equiv} is converted to B_{iso} by the following equation.

Isotropic U_{equiv}: Isotropic U_{equiv} values are converted to isotropic B:

$$B_{iso}[nm^2] = 0.01 \cdot 8.0 \cdot \pi^2 \cdot U_{equiv}$$

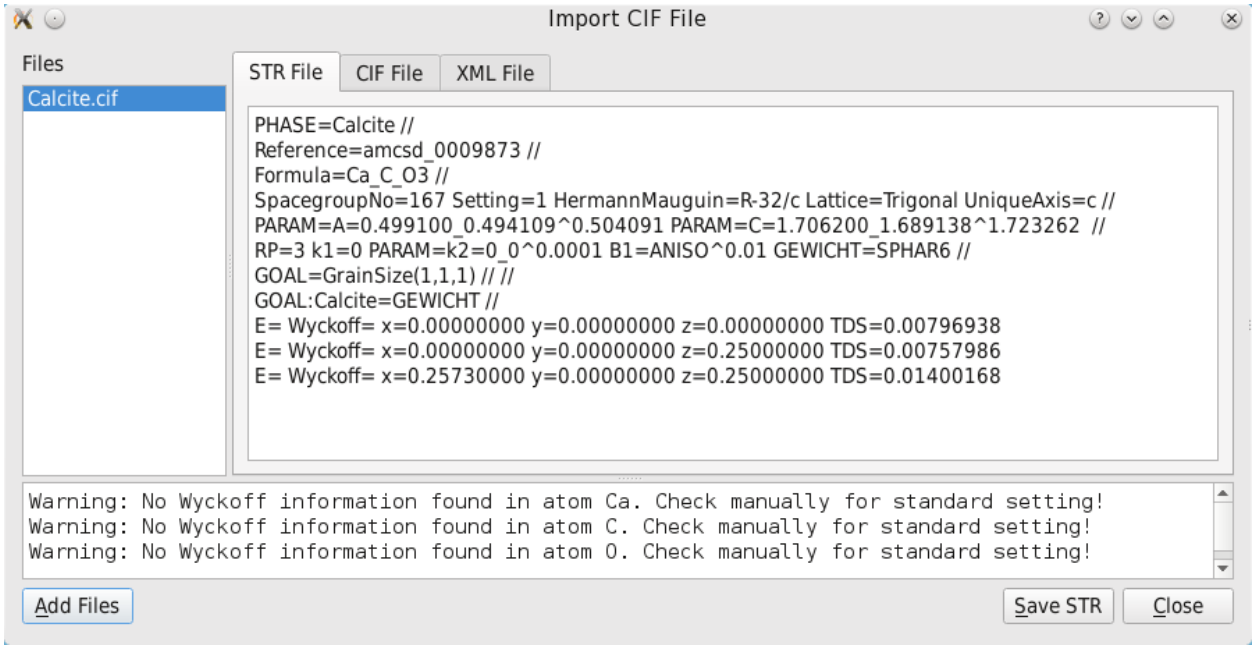

Import CIF File
Files
Calcite.cif
STR File
CIF File
XML File
PHASE=Calcite //
Reference=amcsd_0009873 //
Formula=Ca_C_O3 //
SpacegroupNo=167 Setting=1 HermannMauguin=R-32/c Lattice=Trigonal UniqueAxis=c //
PARAM=A=0.499100_0.494109^0.504091 PARAM=C=1.706200_1.689138^1.723262 //
RP=3 k1=0 PARAM=k2=0_0^0.0001 B1=ANISO^0.01 GEWICHT=SPHAR6 //
GOAL=GrainSize(1,1,1) // //
GOAL:Calcite=GEWICHT //
E= Wyckoff= x=0.00000000 y=0.00000000 z=0.00000000 TDS=0.00796938
E= Wyckoff= x=0.00000000 y=0.00000000 z=0.25000000 TDS=0.00757986
E= Wyckoff= x=0.25730000 y=0.00000000 z=0.25000000 TDS=0.01400168
Warning: No Wyckoff information found in atom Ca. Check manually for standard setting!
Warning: No Wyckoff information found in atom C. Check manually for standard setting!
Warning: No Wyckoff information found in atom O. Check manually for standard setting!
Add Files
Save STR
Close

Figure 14: After importing a CIF file and adding all space group information, the STR file is displayed. It may still be incomplete. Check the warnings at the bottom of the dialog and fix the STR file text manually. The CIF file is also shown in the second tab for comparisong. The XML file in the third tab is only used internally by Profex.

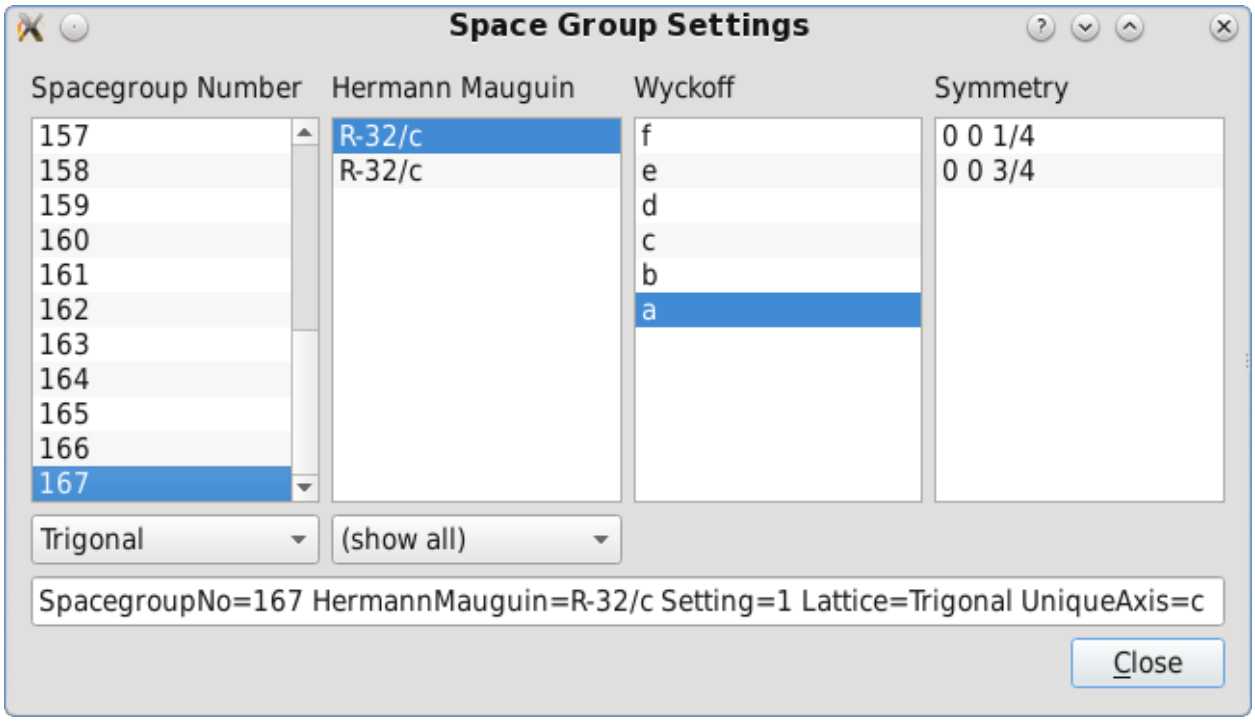


Figure 15: „Help → BGMN SPACEGRP.DAT" opens a dialog to browse all space group numbers, settings, and atomic positions.

CIF File	STR File
_chemical_name_mineral	PHASE=***name***
_chemical_name_common	PHASE=***name***
_chemical_name_systematic	PHASE=***name***
_database_code_[a-z]	Reference=***name***
_chemical_formula_[a-z]	Formula=***name***
_symmetry_Int_Tables_number	SpacegroupNo=***number***
_space_group_IT_number	SpacegroupNo=***number***
_symmetry_space_group_name_H-M	HermannMauguin=***symbol***
_space_group_name_H-M_alt	HermannMauguin=***symbol***
_cell_length_a / _b / _c	A= / B= / C=***value***
_cell_angle_alpha / _beta / _gamma	ALPHA= / BETA= / GAMMA=***value***
_atom_site_label	E=***M*±*n***(*value*)
_atom_site_type_symbol	E=***M*±*n***(*value*)
_atom_site_Wyckoff_symbol	Wyckoff=***symbol***
_atom_site_occupancy	E=*M*±*n*(***value***)
_atom_site_fract_x / _y / _z	x= / y= / z=***value***
_atom_site_B_iso_or_equiv	TDS=***value***
_atom_site_U_iso_or_equiv	TDS=***value***
_atom_site_aniso_U_[1-3]	TDS=***value***
_atom_site_aniso_B_[1-3]	TDS=***value***

Table 2: Assignment of CIF parameter tags to BGMN STR variables.

12. Instrument configurations

Raytraced geometric peak profiles must be calculated by BGMN prior to refinement. The instrument configuration is described in a control file, and the two programs `GEOMET` and `MAKEGEQ`, which are part of the BGMN software distribution, are used to calculate and interpolate the peak profile in a specific 2θ range. For more information please refer to the BGMN documentation [1].

Profex allows editing instrument control files in a simple text editor, and runs `GEOMET` and `MAKEGEQ` to generate the output files. A common workflow to modify an existing device configuration is shown below.

1. Run Profex and click „Instrument → Edit Configuration…". Profex will open a file dialog in the Device database directory. Select the instrument control file (*.sav) you intend to modify.
2. The instrument dialog shown in Fig. 16 will be shown. Edit the file as intended.
3. Save the file under a new name using the dialog's „Save As" button. Be sure to save it in a directory with write access.
4. Check the options „Raytrace (GEOMET)" and „Interpolate (MakeGEQ)". The option „Calculate Profile (GERTEST)" is optional.
5. Click the „Run" button and wait until the progress dialog has completed. Depending on hardware, simulated angular range, and device configuration, this process may take several minutes to complete.

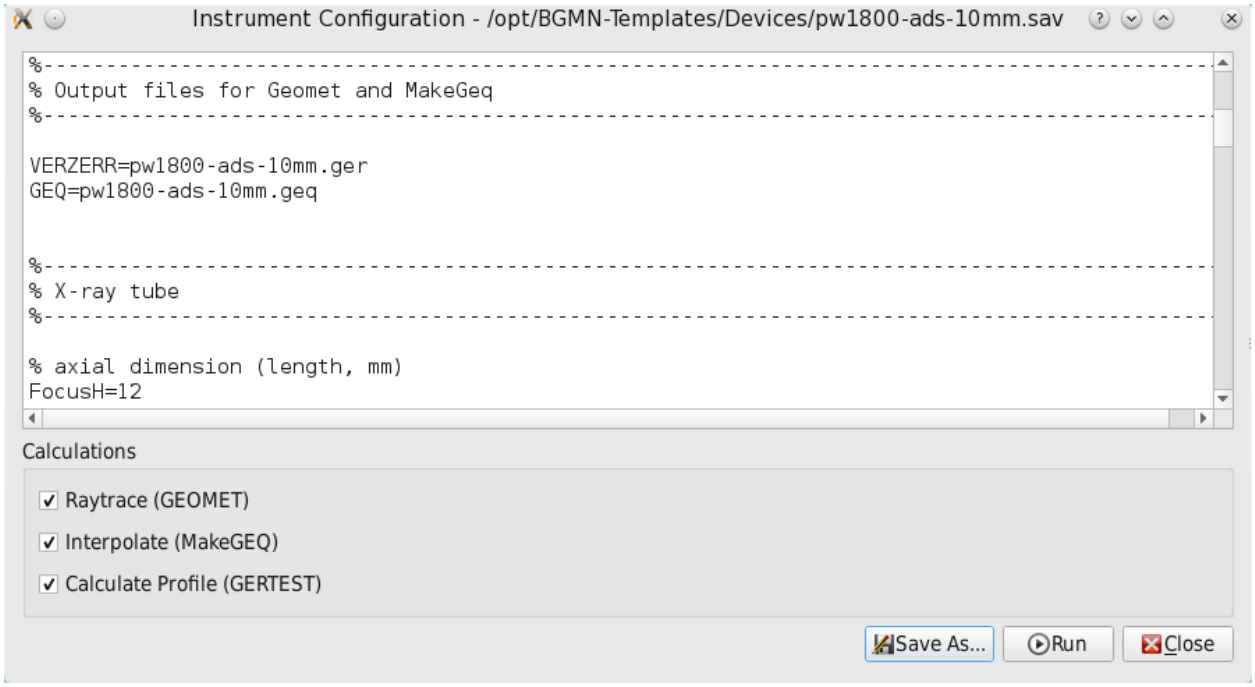


Figure 16: „Instrument → Edit Configuration…" opens a dialog to edit an existing instrument configuration.

Once the process has completed, BGMN has created two new files (*.ger and *.geq), which are required for refinements. If they were created outside of the Device database directory, they should be moved there in order to appear in the ,,Add Phase" dialog. It is also recommended to manually create a template file for the new configuration, as described in section 3.4.3.

Running `GERTEST` will also create a file with the extension *.xy, which contains a simulated pattern with peaks at regular positions. This is convenient for comparing the peak profile shape of different instruments graphically, similar to ,,Tools $\rightarrow$ Show Device Function" in BGMNwin, but otherwise it is of not much use.

13. Scan File Handling

In contrast to the BGMN Rietveld backend, which only supports a limited number of scan file formats natively, Profex reads a wide and growing range of file formats. When running a refinement on a scan file format not supported by BGMN, Profex will by default automatically convert the file in the background and modify the control file accordingly. This section describes the conversion process and the settings allowing the user to control the conversion.

Automatic scan file conversion can be switched on and off in the preferences dialog by checking or unchecking the option „Edit → Preferences... → BGMN → Convert raw scans to XY format". Scan file handling by Profex will be different depending on this setting. Unless conversion is not desired for specific reasons, users are strongly advised to activate this option.

It is a surprisingly complex task to determine the correct file name of a project's raw scan (VAL[n] keyword in the control file). The possible scenarios to be considered are manifold. Profex has sophisticated routines to determine the best guess for a VAL file name under all circumstances. These routines are illustrated in Figures 18–21.

In principle, when creating a new project, a raw scan file as obtained from the instrument is opened and a new control file is created either by using the „Add a new phase" dialog or the „Copy control file" function (see section 4). Either way the loaded raw scan file determines the location and the base name of the project, and all input and output file names in the control file will automatically be set to this scan's file base name. More information on file name handling is given in section 3.4.3. The scan file name to be read by the BGMN Rietveld backend is specified with the `VAL[n]=ScanFile.xxx` line in the control file. The scan file name is given by the project name, as described above, but the file format and extension is determined by Profex automatically, depending on the raw scan format and the setting of „Edit → Preferences... → BGMN → Convert raw scans to XY format". If a format natively supported by BGMN is detected, the file will be used without conversion. If the format is not supported, the behavior will depend on the setting „Convert raw scans to XY format": If active, the file will be converted to *.xy format and the VAL[n] file entry will be adapted accordingly. If inactive, no conversion will be done and it is in the user's responsibility to guarantee correct file names and formats. See Fig. 17 for more explanations.

However, the processes described above represent relatively simple scenarios, when the raw scan file is opened and the format and file name are known. In many situations it gets a lot trickier to determine the correct file name. The following situation represents a worst case: A DIA file is opened, conversion to *.xy is inactive, and the control file is created from another project using the „Copy control file" feature. Normally, when a DIA file exists, a control file should also exist with a valid VAL[n] entry. However, when sharing or moving DIA files, or when the base name of the DIA and control file do not match, it may still occur that a DIA file is present but the corresponding control file cannot be located. Trying to find the correct raw scan file used to create die DIA file is difficult in such a situation:

1. The control file copied over from another project contains input and output file names (VAL, DIAGRAMM, OUTPUT, etc.) of the source project. All file names must be changed to the destination project. The VAL file name found in this control file must not be used.

2. The displayed scan is a DIA file, which cannot be used as input file.

3. Converting the DIA file to *.xy is not allowed.
4. There is no reference to the raw scan in any of the available files.
5. In that case, Profex will scan the directory of the DIA file for a raw scan file in a format natively supported by BGMN. But there is no guarantee that such a file is found.

This is one of many scenarios when finding the correct VAL file name is not trivial. However, the complex processes illustrated in Figures 18–21 cover most situations, and if no solution can be found, a warning will be issued.

If the raw scan format (here: xrdml) is not natively supported by BGMN, Profex will change the VAL[n] file name to *.xy and convert the file automatically.

```
working directory
├── scan_1.sav
├── scan_1.xrdml
├── structure_1.str
├── instrument.sav
├── instrument.geq
└── instrument.ger
```

```
% Input files
VAL[1]=scan_1.xy
VERZERR=instrument.geq
LAMBDA=CU
STRUC[1]=structure_1.str
% Output files
LIST=scan_1.lst
OUTPUT=scan_1.par
DIAGRAMM=scan_1.dia
...
```

If conversion to *.xy is deactivated, VAL[n] will be the raw scan file. If it is not supported natively by BGMN (e. g. xrdml), refinement will not start.

```
working directory
├── scan_1.sav
├── scan_1.xrdml
├── structure_1.str
├── instrument.sav
├── instrument.geq
└── instrument.ger
```

```
% Input files
VAL[1]=scan_1.xrdml
VERZERR=instrument.geq
LAMBDA=CU
STRUC[1]=structure_1.str
% Output files
LIST=scan_1.lst
OUTPUT=scan_1.par
DIAGRAMM=scan_1.dia
...
```

Natively supported file formats (here: Seifert val) do not require conversion to *.xy. Profex will use the raw scan file name for the VAL[n] entry, regardless of the state of the „Convert raw scans to XY" setting.

```
working directory
├── scan_1.sav
├── scan_1.val
├── structure_1.str
├── instrument.sav
├── instrument.geq
└── instrument.ger
```

```
% Input files
VAL[1]=scan_1.val
VERZERR=instrument.geq
LAMBDA=CU
STRUC[1]=structure_1.str
% Output files
LIST=scan_1.lst
OUTPUT=scan_1.par
DIAGRAMM=scan_1.dia
...
```

Figure 17: Some examples for working and failing VAL[n] file scenarios.

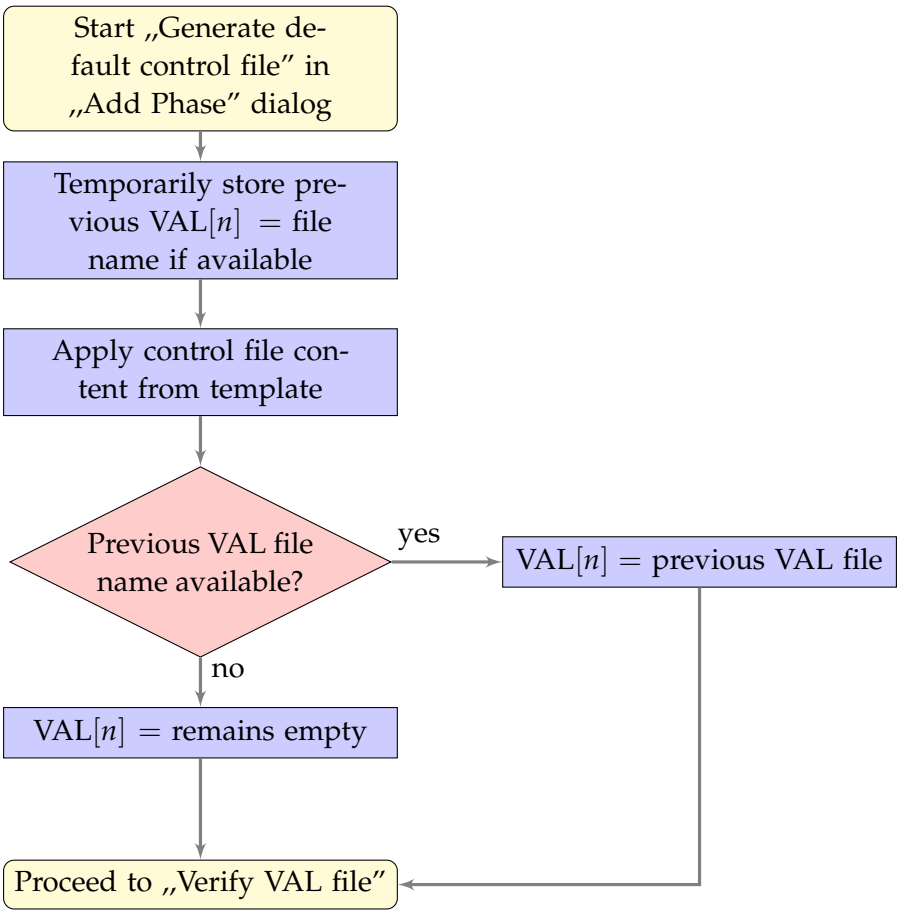

Start „Generate default control file" in „Add Phase" dialog
Temporarily store previous VAL[n] = file name if available
Apply control file content from template
Previous VAL file name available?
yes
VAL[n] = previous VAL file
no
VAL[n] = remains empty
Proceed to „Verify VAL file"

Figure 18: VAL file handling when calling the „Add Phase" dialog and activating the option „Generate default control file" to create a control file from a template file.

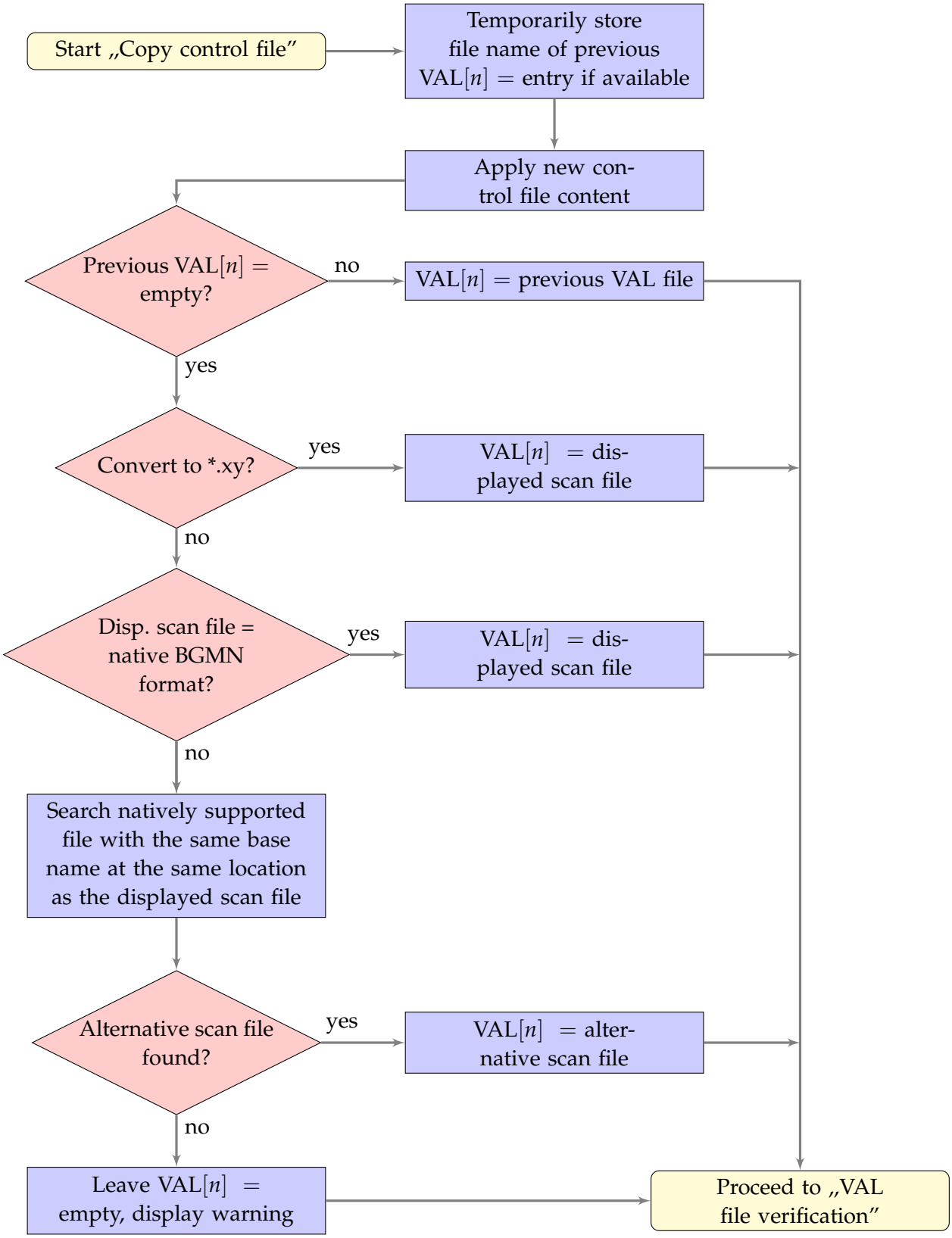

Start „Copy control file”
Temporarily store file name of previous VAL[n] = entry if available
Apply new control file content
Previous VAL[n] = empty?
no
VAL[n] = previous VAL file
yes
Convert to *.xy?
yes
VAL[n] = displayed scan file
no
Disp. scan file = native BGMN format?
yes
VAL[n] = displayed scan file
no
Search natively supported file with the same base name at the same location as the displayed scan file
Alternative scan file found?
yes
VAL[n] = alternative scan file
no
Leave VAL[n] = empty, display warning
Proceed to „VAL file verification”

Figure 19: VAL file name handling when using the „Copy control file” function.

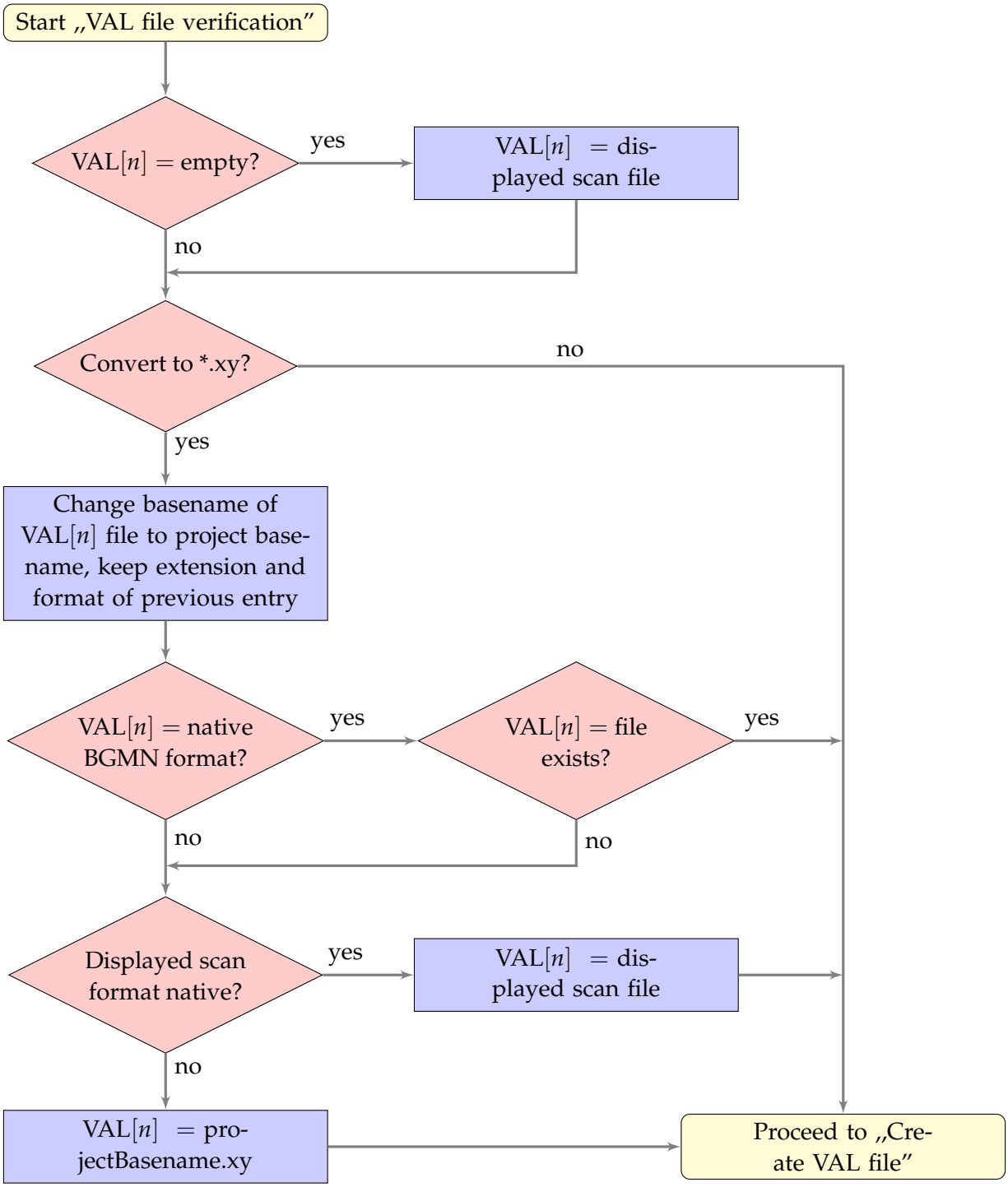


Figure 20: Automatic verification of a VAL[n] file entry in the SAV control file. This function is called at several occasions when modifying the control file content. E. g. after creating a default control file, or after applying a control file from another project.

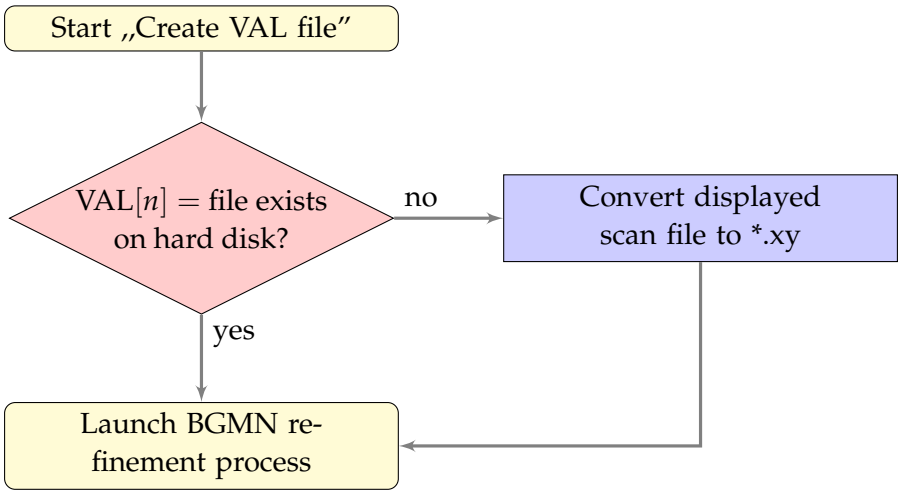


Figure 21: Immediately before running the refinement process, Profex checks whether the VAL file referenced in the control file exists on the hard disk. If not, a *.xy file will be created from the currently displayed scan file.

A. Bundle File Structure

A.1. Windows

```
Profex-BGMN-Bundle-3.3.zip
├─ BGMNwin
│  ├─ BGMN.EXE
│  ├─ MakeGEQ.EXE
│  └─ ...
└─ Profex-3.3
   ├─ Devices
   │  ├─ Instrument 1.sav
   │  ├─ Instrument 1.ger
   │  ├─ Instrument 1.geq
   │  ├─ Instrument 1.tpl
   │  ├─ Instrument 2.sav
   │  └─ ...
   ├─ Structures
   │  ├─ Structure 1.str
   │  ├─ Structure 2.str
   │  └─ ...
   ├─ profex.exe
   └─ ...
```

A.2. Mac OS X

```
Profex-BGMN-Bundle-3.3.dmg
└─ Profex-BGMN
   ├─ profex.app
   ├─ BGMNwin
   │  ├─ bgmn
   │  ├─ makegeq
   │  └─ ...
   └─ BGMN-Templates
      ├─ Devices
      │  ├─ Instrument 1.sav
      │  ├─ Instrument 1.ger
      │  ├─ Instrument 1.geq
      │  ├─ Instrument 1.tpl
      │  ├─ Instrument 2.sav
      │  └─ ...
      └─ Structures
         ├─ Structure 1.str
         ├─ Structure 2.str
         └─ ...
```

A.3. Linux

No bundle is available for Linux.

References

[1] http://www.bgmn.de/

[2] https://www.ill.eu/sites/fullprof/

[3] http://profex.doebelin.org/

[4] http://qt-project.org/

[5] http://quazip.sourceforge.net/

[6] http://support.apple.com/kb/ht3696/

[7] http://www.iucr.org/resources/cif/spec/version1.1/cifsyntax/

[8] http://users.uoi.gr/nkourkou/powdll/

[9] http://fityk.nieto.pl/

[10] Fischer, R.X., Tillmanns, E. *The equivalent isotropic displacement factor.* Acta Cryst. C44, 1988, 775–776.

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